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December 13, 2001

Ms. Christine Todd Whitman, Administrator  
U.S. Environmental Protection Agency  
P.O. Box 1473  
Merrifield, VA 22116

Subject: High Production Volume (HPV) Chemical Challenge Program – Test  
Plan Submission Consortium Registration No.

Dear Governor Whitman:

The American Chemistry Council's Phosphoric Acid Derivatives Panel submits for review and public comment its test plan, as well as related robust summaries, for the "Phosphoric Acid Derivatives" category of chemicals under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program. The Panel understands that there will be a 120-day review period for the test plan and that all comments generated by or provided to EPA will be forwarded to the Panel for consideration.

Relying on several factors specified in EPA's guidance document on "Development of Chemical Categories in the HPV Challenge Program," in which use of chemical categories is encouraged, the following closely related chemicals constitute the "Phosphoric Acid Derivatives" category:

Tris(2-ethylhexyl) phosphate (78-42-2)  
2-Ethylhexyl phosphate (12645-31-7)  
Dibutyl hydrogen phosphate (107-66-4)\*  
Tributyl phosphate (126-73-8)\*  
Bis(2-ethylhexyl) hydrogen phosphate (298-07-7)\*

Please note that the chemicals marked with an asterisk are not sponsored as part of the EPA HPV Challenge Program and are used for data purposes only.

The Panel has given careful consideration to the animal welfare principles contained in the EPA's October 14, 1999, letter to HPV Challenge Program participants. As directed, the Panel has sought to maximize the use of existing data for scientifically appropriate related chemicals and structure-activity-relationships. Additionally, the Panel has conducted a thoughtful, qualitative analysis rather than use a rote checklist approach in analyzing the adequacy of existing data.

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The Panel intends to fulfill all the Screening Information Data Set (SIDS) endpoints of the HPV program through the use of existing data. In addition, some endpoints have been completed through the utilization of data from studies conducted on structurally similar compounds and from modeling programs accepted by the EPA. The Panel believes these data are adequate to satisfy the requirements of the HPV program without the need for new or additional tests.

Dr. Susan Anderson Lewis of my staff is the technical contact for this Panel. Should you have any questions or comments, please contact her at 703-741-5635 (Phone), 703-741-6091 (Fax) or [susan\\_lewis@americanchemistry.com](mailto:susan_lewis@americanchemistry.com) (e-mail).

Sincerely yours,

Courtney M. Price  
Vice President, CHEMSTAR

Attachments

CC: O. Hernandez, EPA  
C. Auer, EPA  
Phosphoric Acid Derivatives Panel  
Steven Russell, ACC  
Jim Keith, ACC

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**Phosphoric Acid Derivatives  
Category Justification and Testing Rationale**

**CAS Nos. 78-42-2 and 12645-31-7 (HPV Chemicals)  
107-66-4, 126-73-8 and 298-07-7 (Supporting Chemicals)**

**Phosphoric Acid Derivatives Panel  
American Chemistry Council**

**December, 2001**

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**List of Member Companies in the Phosphoric Acid Derivatives Panel**

The Phosphoric Acid Derivatives Panel of the American Chemistry Council includes the following member companies: Baker Petrolite Corporation, Bayer Corporation, Noveon, Inc. (formerly BF Goodrich), Crompton Corporation, and ICI Americas (Uniqema).

**Executive Summary**

The American Chemistry Council's Phosphoric Acid Derivatives (PAD) Panel, and its member companies, hereby submit for review and public comment their test plan for the Phosphoric Acid Derivatives category of chemicals under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program.

As discussed in the report that follows, PAD chemicals are used primarily as flame retardant plasticizers for polyvinylchloride resins, cellulose esters, lacquers and plastics, contributing flexibility and resistance to degradation at low temperatures. They are used as solvents in liquid-liquid extractions, and as intermediates for wetting agents and detergents, as well as anti-foaming agents. They are used extensively as dispersing agents in plastisols, as catalysts in the manufacture of phenolic and urea resins, and in metal separation and extraction. These chemicals are also used as heat exchange mediums (2000 Chemical Economics Handbook).

All chemicals in this category are alkyl esters of phosphoric acid and have been reviewed by the GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance (BUA, 1992) as a category. Existing data for members of this category indicate that they are of low concern for aquatic and mammalian toxicity, will partition to soil and sediment, and are not readily biodegradable. We conclude that there is sufficient data on the members of this category to meet requirements of the HPV Challenge Program and no additional testing is proposed.

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## Phosphoric Acid Derivatives Category

Relying on several factors specified in EPA's guidance document on "Development of Chemical Categories in the HPV Challenge Program," in which use of chemical categories is encouraged, the following closely related chemicals constitute a chemical category:

Tris(2-ethylhexyl) phosphate	(78-42-2)
2-Ethylhexyl phosphate	(12645-31-7)
Dibutyl hydrogen phosphate	(107-66-4)*
Tributyl phosphate	(126-73-8)*
Bis(2-ethylhexyl) hydrogen phosphate	(298-07-7)*

*\*Not sponsored as part of the EPA HPV Challenge Program. Used for data purposes only.*

### Structural Similarity.

A key factor supporting the classification of these chemicals as a category is their structural similarity. All chemicals in this category are alkyl esters of phosphoric acid (See **Figure 1**). The GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance reviewed the alkyl phosphate esters as a category in 1992 (BUA, 1992).

### Metabolism.

"In mammalian metabolism, the phosphoric acid tri-esters are, as a rule, rapidly degraded to the corresponding di-ester. Only a small amount is further metabolized to the monophosphates" (BUA, 1992).

### Conclusion.

In consideration of animal welfare concerns to minimize the use of animals in the testing of chemicals, the Panel has conducted a thorough literature search for all available data, published and unpublished. It has performed an analysis of the adequacy of the existing data. Further, it developed a scientifically supportable category of related chemicals and used structure-activity relationship information to address certain requirements. The use of animals in this proposed test plan has been minimized.

Based upon the data provided in this report and the attached IUCLID documents, the physicochemical and toxicological properties of the PAD category members are similar and follow a regular pattern as a result of that structural similarity. Therefore, the EPA definition of a chemical category has been met.

All endpoints of the category have adequately satisfied requirements of the HPV Chemical Challenge Program, therefore additional tests are not proposed.

The summary endpoint matrix is included as **Table 5** of this document.

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## Introduction

A provision for the use of categories to reduce testing needs is included under EPA's HPV Program. Specifically, categories may be formed based on structural similarity, through analogy, or through a combination of category and analogy for use with single chemicals. The benefits of using a category approach are numerous and include: accelerated release of hazard information to the public; reduction in the number of animals used for testing; and an economic savings as a result of a reduced testing program.

The PAD chemicals that form this category, arranged in order of increasing molecular weight, are:

<b>2-Ethylhexyl phosphate</b>	<b>(12645-31-7)</b>
Dibutyl hydrogen phosphate	(107-66-4) *
Tributyl phosphate	(126-73-8) *
Bis (2-ethylhexyl) hydrogen phosphate	(298-07-7) *
<b>Tris (2-ethylhexyl) phosphate</b>	<b>(78-42-2)</b>

Two chemicals are sponsored by this Panel in the US EPA HPV Program. The chemicals marked with an asterisk (\*) are included in support of the category, however are not being sponsored by this Panel. CAS # 107-66-4 and #126-73-8 have been assessed through the OECD SIDS Program. CAS# 298-07-7 will be sponsored by American Chemistry Council's HERTG Panel in 2003.

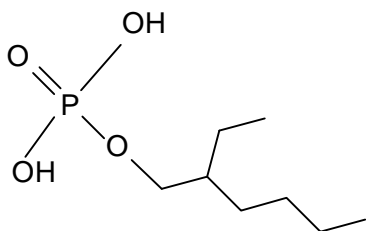
## Development of the Phosphoric Acid Derivatives Category

EPA has described a stepwise process for developing categories. These steps include:

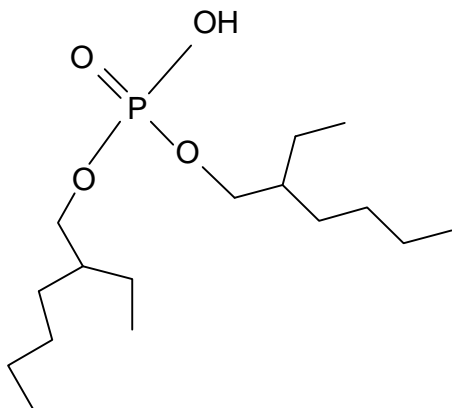
- Grouping a series of like chemicals, including the definition of criteria for the group.
- Gathering data on physicochemical properties, environmental fate and effects, and health effects for each member of the category.
- Evaluating the data for adequacy.
- Constructing a matrix of available and unavailable data.
- Determining whether there is a correlation among category members and data gathered.

## Definition of the Phosphoric Acid Derivatives Category

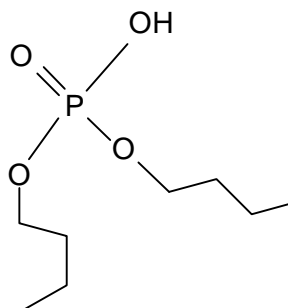
As defined by EPA under the HPV Program, a chemical category is "a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity." The similarities should be based on a common functional group, common precursors or breakdown products (resulting in structurally similar chemicals) and an incremental and constant change across the category. The goal of developing a chemical category is to use interpolation and/or extrapolation to assess chemicals rather than conducting additional testing.



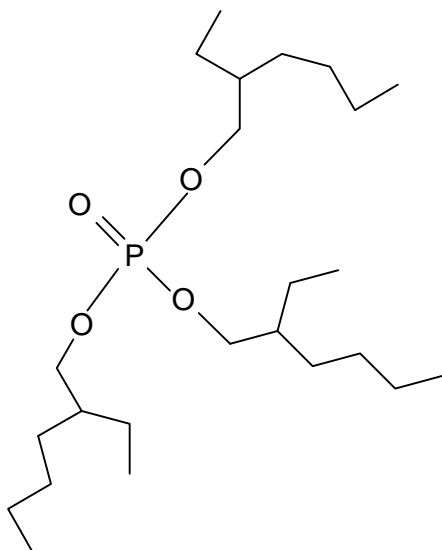
**2-ethyl hexyl phosphate**  
CAS # 12645-31-7



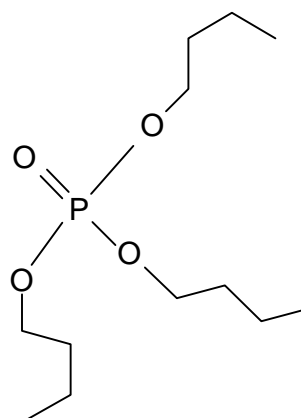
**bis (2-ethyl hexyl) phosphate**  
CAS # 298-07-7



**dibutyl hydrogen phosphate**  
CAS # 107-66-4



**tris (2-ethyl hexyl) phosphate**  
CAS # 78-42-2



**tributyl phosphate**  
CAS # 126-73-8

**Figure 1. Chemical Structures**

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## Structural Similarity.

A key factor supporting the classification of these chemicals as a category is their structural similarity. The chemicals within the PAD category are defined as esters of phosphoric acid, having a phosphoric acid backbone with various alkyl substituents as illustrated in **Figure 1**. The GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance reviewed the alkyl phosphate esters as a category in 1992 (BUA, 1992).

## Metabolism.

“In mammalian metabolism, the phosphoric acid tri-esters are, as a rule, rapidly degraded to the corresponding di-ester. Only a small amount is further metabolized to the monophosphates.” (BUA, 1992). In the case of tributyl phosphate, dibutyl hydrogen phosphate was the major metabolite (40-64% of the identified dose) and butyl dihydrogen phosphate was measured as 11-21% of the identified dose (Suzuki et al., 1984; IUCLID data set on CAS# 126-73-8).

## Matrix of SIDS Endpoints

In order to construct a matrix of SIDS endpoints for the members of the PAD category, the data on physicochemical properties, environmental fate, ecotoxicity and health effects for each member of the category was collected and evaluated for adequacy. The results of these activities are presented in the tables and text below, as well as the attached IUCLID documents, providing a matrix of available data.

## Correlation of Physicochemical Properties

The physicochemical properties of the members of the PAD category are presented in **Table 1**. The PAD chemicals are non-flammable, colorless or pale colored liquids with low water solubility, very low vapor pressure and low partition coefficients. The similarities in the other physicochemical properties of these chemicals are explained by similarities in their chemical structure, and provide justification of this group of chemicals as a category within the HPV Challenge Program.

All members of the category have measured or calculated data on physicochemical properties. Data is available on all physicochemical endpoints for this category (See **Table 1**), therefore the requirements of the HPV Chemical Challenge Program have been adequately satisfied.

## Correlation of Environmental Fate

The HPV Challenge Program requires that hydrolysis, photodegradation, biodegradation and environmental transport information be presented for each chemical or bridged to each member of a category. The EPIWIN modeling Program was used to calculate the photodegradation and fugacity for each chemical in the category. Two chemicals have been tested for photodegradation and there is good correlation with the calculated results. The members of this category have short photodegradation half-lives.

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Adequate biodegradation data exist for four of the chemicals in this category; bridging will be used to fill the remaining requirement. Two chemicals (126-73-8 and 298-07-7) are categorized as “readily biodegradable” with degradation rates > 70% in the “ready test”. Two chemicals (107-66-4 and 78-42-2) are regarded as “not readily biodegradable” with rates < 60% in the “closed bottle” test. The trend within the closed bottle tests clearly showed that the compound is metabolized slower as it becomes more polar. Thus, one could predict that the mono-ester would not be metabolized in the “closed bottle” system. The mono-ester (#12645-31-7) is expected to be “not readily biodegradable”.

Partitioning to soil and sediment fractions (vs. water and air) is expected according to Fugacity Level III calculations. Default “input values” of 1000 kg/hr were used for the modeling.

Data is available or bridged for all Environmental Fate endpoints for this category (See **Table 2**), therefore the requirements of the HPV Chemical Challenge Program have been adequately satisfied.

### **Correlation of Ecotoxicity**

The HPV Challenge Program requires that an acute aquatic toxicity test in fish, invertebrates, and algae be performed or bridged to each member of a category. Existing data indicate that the members of the PAD category have low water solubility. The low water solubility suggests that the acute aquatic toxicity of these chemicals should be low due to limited bioavailability to aquatic organisms. In general, data and modeling (ECOSAR) results support the low toxicity of PAD chemicals to aquatic organisms (See **Table 3**).

Data for the bis- and tris-(2-ethyl hexyl) esters demonstrate 96 hr Acute Fish LC<sub>50</sub> from 30 mg/l to >100 mg/l. ECOSAR estimation for CAS#12645-31-7 is in line with the measured data.

Calculated and actual data for the mono- and bis-(2-ethyl hexyl) esters demonstrate 48 hr Acute Invertebrate LC<sub>50</sub> to be >42 mg/l. Since the mono phosphate is expected to be more toxic than the tris-ester, the acute *Daphnia* LC<sub>50</sub> of tris-(2-ethyl hexyl) phosphate is predicted to be >42 mg/l.

Acute toxicity to algae has been tested for 2-ethyl hexyl phosphate (12645-31-7) and demonstrated an EC<sub>50</sub> of 161-168 mg/l. Since the mono phosphate is expected to be more toxic than the bis- and tris-esters, the EC<sub>50</sub> of the tris-ester is expected to be greater than or equal to 161 mg/l.

No additional aquatic toxicity tests are proposed for this category as data is available or bridged for all endpoints (See **Table 3**). The requirements of the HPV Chemical Challenge Program have been adequately satisfied.

### **Correlation of Health Effects**

#### **Acute Mammalian Toxicity**

Acute oral, dermal and inhalation toxicity data for the category is summarized in **Table 4**. Of the chemicals tested, all show a very low order of toxicity following oral or dermal administration. Although not all reports are GLP, may not follow OECD Guidelines, or may not be “robust” in their summaries, the “weight of evidence” demonstrates the low concern for acute toxicity.

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The similarity in the order of toxicity for these chemicals is consistent with their similar chemical structure, metabolism, and physicochemical properties and supports the scientific justification of these chemicals as a category within the HPV Challenge Program. The acute oral LD<sub>50</sub> of 2-Ethyl hexyl phosphate (12645-31-7) is expected to be about 2000 mg/kg bw in rats, which is similar to the acute toxicity of Dibutyl hydrogen phosphate (107-66-4) of same molecular weight.

The dermal LD50 for tributyl phosphate and tris(2-ethyl hexyl) phosphate are > 10,000 mg/kg bw. It is predicted that the acute dermal toxicity of 2-ethyl hexyl phosphate will also be in the non-toxic range.

The HPV Challenge Program requires that either an acute test be performed or bridged to each member of a category. Adequate acute oral toxicity tests exist for four of the five PAD chemicals. By bridging existing data to the one chemical where no data was found, the requirements of the HPV Challenge Program with respect to acute toxicity endpoints has been met, and no additional acute toxicity testing is proposed.

### **Repeat Dose Toxicity**

A summary of the repeat dose toxicity data for the PAD category is presented in **Table 4**.

Repeat dose studies (28 D and/or 90 D studies) have been conducted with three of the PAD chemicals and demonstrate an apparent reduction in toxicity with increasing molecular weight. The repeat dose toxicity of 2-ethyl hexyl phosphate (12645-31-7) is expected to be similar to the repeat dose toxicity of Dibutyl hydrogen phosphate (107-66-4) of same molecular weight. The 44 day oral exposure NOAEL of Dibutyl hydrogen phosphate is 30 mg/kg bw in rats.

By bridging existing data to the one chemical where no data was found, the requirements of the HPV Challenge Program with respect to the repeat dose toxicity endpoint has been met, and no additional repeat dose toxicity testing is proposed.

### **Mutagenicity**

A summary of the mutagenicity information for the PAD category is presented in **Table 4**. The weight of evidence for the members of this category indicates these chemicals are not mutagenic or clastogenic.

The HPV Challenge Program requires that adequate bacterial mutagenicity tests and *in vitro* chromosome aberration tests or *in vivo* micronucleus tests be performed or bridged to each member of a category. Adequate bacterial mutagenicity tests exist for four of the five PAD chemicals, and adequate *in vitro* or *in vivo* mammalian studies exist for three of the five chemicals. By bridging existing data to the one chemical where no data was found, the requirements of the HPV Challenge Program with respect to the mutagenicity endpoint has been met, and no additional mutagenicity testing is proposed.

### **Reproductive and Developmental Toxicity.**

A summary of the reproductive and developmental toxicity data for the PAD category is presented in **Table 4**.

Adequate reproductive and developmental studies are available for two of the lower molecular weight chemicals in this category. These studies indicate an absence of reproductive or developmental effects of

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these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, bridging existing data to the chemicals where no data was found is acceptable. No reproductive or developmental effects of 2-ethyl hexyl phosphate (12645-31-7) or tris (2-ethyl hexyl) phosphate (78-42-2) is expected at doses ranging from >225 to 1000 mg/kg.

By bridging existing data to the chemicals where no data was found, the reproductive and developmental toxicity aspect of this category has been evaluated adequately, meeting the requirements of the HPV Challenge Program and no additional reproductive and developmental toxicity testing is proposed.

### **Summary Endpoint Matrix / Test Plan**

All endpoints of the category have been adequately characterized, meeting the requirements of the HPV Challenge Program, therefore additional tests are not proposed. A summary endpoint matrix is included as **Table 5** of this document.

### **Background Information: Manufacturing and Commercial Applications**

#### **Manufacturing**

Tris (2-ethyl hexyl) phosphate (78-42-2) is produced by the reaction of phosphorus oxychloride with 2-ethyl hexanol followed by removal of hydrogen chloride co-product and typically further purification steps.

#### **Commercial Applications**

PAD chemicals are used as flame retardant plasticizers for polyvinylchloride resins, cellulose esters, lacquers and plastics, contributing flexibility and resistance to degradation at low temperatures, as solvents in liquid-liquid extractions, and as intermediates for wetting agents and detergents, as well as anti-foaming agents. They are used extensively as dispersing agents in plastisols, as catalysts in the manufacture of phenolic and urea resins, and in metal separation and extraction. These chemicals are also used as heat exchange mediums. (2000 Chemical Economics Handbook)

#### **Shipping/Distribution**


PAD chemicals are shipped extensively throughout the world from manufacturing plants.

#### **Worker/Consumer Exposure**

The Phosphoric Acid Derivatives industry has a long safety record and sophisticated users handle these chemicals. Exposure of workers handling PAD materials is likely to be highest in the area of packaging. These materials are liquids of very low vapor pressure, thus during the packaging process there is a low potential for inhalation exposure; an exposure of workers - if any- could take place by inhalation of very small droplets. Depending on handling procedures and filling equipment, dermal contact to the liquid is also possible.

**Table 1. Matrix of Available and Adequate Data on the Phosphoric Acid Derivatives Category  
Physico-chemical Properties**


<b>Chemical</b>	<b>2-Ethyl hexyl phosphate</b>	<b>Dibutyl hydrogen phosphate</b>	<b>Tributyl phosphate</b>	<b>Bis (2-ethyl hexyl) phosphate</b>	<b>Tris (2-ethyl hexyl) phosphate</b>
<b>CAS#</b>	<b>12645-31-7</b>	<b>107-66-4</b>	<b>126-73-8</b>	<b>298-07-7</b>	<b>78-42-2</b>
<b>Molecular Weight:</b>	210.21	210.21	266.32	322.43	434.65
<b>Physical State</b>	Colorless liquid	Pale, amber liquid	Colorless liquid	amber liquid	Colorless liquid
<b>Melting Point</b>	81.3°C (EPI)	-13°C 59.33°C (EPI)	< -70°C 64.73 °C (EPI)	-50°C 86.3°C (EPI)	< -70°C 87°C (EPI)
<b>Boiling Point</b>	(decomp)  354°C @ 1013 hPa (EPI)	>200°C @ 20 hPa  319°C @ 1013 hPa (EPI)	130°C @ 5 hPa  327°C @ 1013 hPa (EPI)	240°C @ 1013 hPa (decomp)  400°C @ 1013 hPa (EPI)	>210°C @ 5 hPa (decomp)  446°C @ 1013 hPa (EPI)
<b>Relative Density</b>	1.05 g/cm <sup>3</sup> @ 20°C	1.05 g/cm <sup>3</sup> @ 20°C	0.97 g/cm <sup>3</sup> @ 20°C	0.96 g/cm <sup>3</sup> @ 20°C	0.92 g/cm <sup>3</sup>
<b>Vapor Pressure</b>	7.12 x10(-7)hPa @25°C (EPI)	2.42 x 10(-5) hPa @25°C (EPI) < .1 hPa at 20 ° C	3.47 x 10(-6) hPa @25°C	6.199 x10(-8) hPa @25°C (EPI)	2.05 x 10(-7)hPa @25°C (EPI)
<b>Partition Coefficient (logP<sub>ow</sub>)</b>	2.65 (EPI)	0.6-1.4  2.2 (EPI)	2.5  3.8 (EPI)	4.6-5.4 (ClogP)  6.071 (EPI)	4.2  9.49 (EPI)
<b>Water Solubility</b>	Dispersable  211 mg/l @25°C (EPI)	18 g/l @20°C  430 mg/l @25°C (EPI)	0.4 g/l @20°C  7.35 mg/l @25°C (EPI)	< 1 g/l  0.059 mg/l @25°C (EPI)	2 mg/l  < 0.01 mg/l @25°C (EPI)

 = Non-sponsored chemicals used for data purposes only

EPI = EPIWIN modeling Program. Meylan, W. and Howard, P. (1999)

**Table 2. Matrix of Available and Adequate Data on the Phosphoric Acid Derivatives Category Environmental Fate**


Endpoint	2-Ethyl hexyl phosphate 12645-31-7	Dibutyl hydrogen phosphate 107-66-4	Tributyl phosphate 126-73-8	Bis (2-ethyl hexyl) phosphate 298-07-7	Tris (2-ethyl hexyl) phosphate 78-42-2
Photodegradation	T ½ = 3.9 hrs (AOP)	T ½ = 2.4 hrs (AOP)	T ½ = 1.6 hrs (AOP) 85% after 1 hr (UV)	T ½ = 2 hrs (AOP)	T ½ = 1.3 hrs (AOP) 80% after 1 hr (UV)
Hydrolysis	Not soluble enough to test	No data found	No hydrolysis after 30 D at any pH	No data found	No data found
Biodegradation	No data found	12% after 28D	77-92% after 28 D	0% after 5 D 75% after 28D (related to O <sub>2</sub> demand)	0% after 28 D
Fugacity Level III			( Level I)		
Air (%)	<0.1	0.183	.0737 (11)	0.278	0.312
Water (%)	29	34.4	41 (58)	12.9	10.9
Soil (%)	70.8	65.3	56.7 (16)	36.7	31.2
Sediment (%)	0.188	0.112	1.52 (15)	50.1	57.6

 = Non-sponsored chemicals used for data purposes only

AOP = AOP Program, version 1.89. EPIWIN modeling Program.  
Meylan, W. and Howard, P. (1999)

**Table 3. Matrix of Available and Adequate Data on the Phosphoric Acid Derivatives Category Ecotoxicity**


Endpoint	2-Ethyl hexyl phosphate 12645-31-7	Dibutyl hydrogen phosphate 107-66-4	Tributyl phosphate 126-73-8	Bis (2-ethyl hexyl) phosphate 298-07-7	Tris (2-ethyl hexyl) phosphate 78-42-2
Acute Fish Toxicity 96 hr LC50	Freshwater fish = <b>38 mg/l</b> (ECOSAR)	<i>B. rerio</i> = <b>&gt;100 mg/l</b> <i>B. rerio</i> = <b>&gt;10,000mg/l</b>	<i>O. mykiss</i> = <b>13 mg/l</b> <i>B. rerio</i> = <b>10-14 mg/l</b>	<i>B. rerio</i> = <b>&gt;56 mg/l</b> <i>S. gairdneri</i> = <b>30 mg/l</b>	<i>B. rerio</i> = <b>&gt;100 mg/l</b> <i>O. latipes</i> = <b>&gt;500 mg/l</b> (48 hr)
Acute Invertebrate Toxicity 48 hr EC50	<i>D. magna</i> = <b>42.7 mg/l</b> (ECOSAR)	<i>D. magna</i> = <b>90.9 mg/l</b> (ECOSAR)	<i>D. magna</i> = <b>2.6 – 9.0 mg/l</b>	<i>D. magna</i> = <b>&gt; 42 mg/l</b>	No data found
Algal Toxicity 96 hr EC50	<i>S. capricornutum</i> = <b>161 - 168 mg/l</b> (72 hr) Green algae = 27.759 mg/l (ECOSAR)	Green algae = <b>57.8 mg/l</b> (ECOSAR)	<i>S. capricornutum</i> = <b>4.4 mg/l</b>	No data found	No data found

 = Non-sponsored chemicals used for data purposes only

ECOSAR = ECOSAR v0.99e. EPIWIN modeling Program. Meylan, W. and Howard, P. (1999)

**Table 4. Matrix of Available and Adequate Data on the Phosphoric Acid Derivatives Category Mammalian Toxicity**

Endpoint	2-Ethyl hexyl phosphate 12645-31-7	Dibutyl hydrogen phosphate 107-66-4	Tributyl phosphate 126-73-8	Bis (2-ethyl hexyl) phosphate 298-07-7	Tris (2-ethyl hexyl) phosphate 78-42-2
Acute Toxicity					
Oral LD50	No data found	<b>2000 mg/kg bw</b> (rat)	<b>1390-11,265</b> <b>mg/kg bw</b> (rat)	<b>4940 mg/kg bw</b> (rat)	<b>&gt;36,800 mg/kg bw</b> (rat) <b>46,000 mg/kg bw</b> (rabbit)
Dermal LD50	No data found	No data found	<b>&gt;3,100 - &gt;10,000</b> <b>mg/kg bw</b> (rabbit)	No data found	<b>~20,000 mg/kg bw</b> (rabbit)
Inhalation LC50	No data found	No data found	<b>&gt;4.242 mg/l</b> (4 hr) (rat) <b>&gt;42 mg/l</b> (6 hr) (rat)	No data found	<b>&gt;0.447 mg/l</b> (4 hr) (rat)
Repeated Dose  NOAEL=	No data found	<b>30 mg/kg</b> (oral – rat- 44 D)	<b>75 mg/kg bw</b> (female) <b>15 mg/kg bw</b> (male) (oral – rats -13 wk)	No data found	<b>1000 mg/kg bw</b> (oral - rat -13 wk) <b>430 mg/kg bw</b> (oral- rat - 30 D) <b>1.6 mg/m<sup>3</sup></b> (inhal. -g.pig- 90D)
Mutagenicity – gene mutation	No data found	Ames – negative	Ames – negative (5 studies - negative 1 study = positive) <i>E. coli</i> - negative Gene mutation (CHO cells) - negative	Ames – negative	Ames – negative mouse lymphoma assay – negative
Mutagenicity – chromosome aberration	No data found	Chrom Aber. (CHL cells) – negative Micronucleus test (mouse)- negative	Chrom Aber. (CHO cells) – negative In vivo Cytogenetic assay (rat) – negative <i>Drosophila</i> SLRL - negative	No data found	Chrom Aber. (CHO cells) – negative Sister chromatid exchange - negative
Reproductive Toxicity	No data found	No effects on repro parameters up to <b>1000mg/kg</b> <b>bw</b> (oral – rat)	No effects on repro parameters up to <b>225 mg/kg bw</b> (oral – rat)	No data found	No data found
Developmental Toxicity NOAEL =	No data found	<b>300 mg/kg bw</b> (oral – rat) (Repro study)	<b>&gt;250 mg/kg bw</b> (oral – rat)	No data found	No data found

 = Non-sponsored chemicals used for data purposes only

**Table 5. Summary of data for the Phosphoric Acid Derivatives Category**

Endpoint	2-Ethyl hexyl phosphate 12645-31-7	Dibutyl hydrogen phosphate 107-66-4	Tributyl phosphate 126-73-8	Bis (2-ethyl hexyl) phosphate 298-07-7	Tris (2-ethyl hexyl) phosphate 78-42-2
<b>Environmental Fate</b>					
Photodegradation	C	C	A	C	A
Hydrolysis	A	NR	A	NR	R
Biodegradability	R	A	A	A	A
Fugacity	C	C	C	C	C
<b>Ecotoxicology</b>					
Acute Fish Toxicity	C	A	A	A	A
Acute Invertebrate Toxicity	C	C	A	A	R
Algal Toxicity	A	C	A	NR	R
<b>Mammalian Toxicology</b>					
Acute Toxicity	R	A	A	A	A
Mutagenicity – gene mutation	R	A	A	A	A
Mutagenicity – chromosome aberration	R	A	A	NR	A
Repeated Dose	R	A	A	NR	A
Reproductive Toxicity	R	A	A	NR	R
Developmental Toxicity	R	A	A	NR	R


**Key for symbols in table:**

A = Adequate data available

R = Endpoint requirement fulfilled using category approach, SAR

C = Endpoint requirement fulfilled based on calculated data

NR = No testing required; chemical not sponsored

 = Non-sponsored chemicals used for data purposes only.

---

## References.

2000 Chemical Economics Handbook, SRI International.

BUA Report. (1992) Existing Chemicals of Environmental Relevance III.  
Beratergremium für Umweltrelevante Altstoffe.

ECOSAR. EPIWin Modeling Program. Meylan W. and Howard P. (1999)  
Syracuse Research Corporation. Environmental Science Center,  
6225 Running Ridge Road, North Syracuse, NY 13212-2510.

Meylan W. and Howard P. (1999) EPIWin Modeling Program.  
Syracuse Research Corporation. Environmental Science Center,  
6225 Running Ridge Road, North Syracuse, NY 13212-2510.

Suzuki et al. (1984). J. Agric. Food Chem. 32: 603-610.

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2001 DEC 14 PM 3:02

## I U C L I D

## D a t a S e t

Existing Chemical ID: 78-42-2  
CAS No. 78-42-2  
EINECS Name tris(2-ethylhexyl) phosphate  
EINECS No. 201-116-6  
TSCA Name Phosphoric acid, tris(2-ethylhexyl) ester  
Molecular Formula C24H51O4P

## Producer Related Part

Company:  
Creation date: 15-JUL-1999

## Substance Related Part

Company:  
Creation date: 15-JUL-1999

Memo: Phosphoric Acid Derivatives Panel

Printing date: 28-NOV-2001  
Revision date:  
Date of last Update: 28-NOV-2001

Number of Pages: 34

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7  
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4  
Flags (profile): Flags: without flag, confidential, non confidential, WGK  
(DE), TA-Luft (DE), Material Safety Dataset, Risk  
Assessment, Directive 67/548/EEC, SIDS

1. General Information

---

## 1.0.1 OECD and Company Information

Type: lead organisation  
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Phosphoric Acid Derivatives Panel  
Street: Wilson Boulevard  
Town: 22209 Arlington, VA  
Country: United States  
Phone: 703-741-5600  
Telefax: 703-741-6091

16-OCT-2001

Type: cooperating company  
Name: Bayer Corporation  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: Baker Petrolite Corporation  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: Crompton Corporation  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: ICI Americas (Uniqema)  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: Noveon, Inc. (formerly BF Goodrich)  
Country: United States

16-OCT-2001

## 1.0.2 Location of Production Site

-

## 1.0.3 Identity of Recipients

-

## 1.1 General Substance Information

-

1. General Information

---

1.1.0 Details on Template

-

1.1.1 Spectra

-

1.2 Synonyms

-

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

-

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

-

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

-

1.9 Source of Exposure

-

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1. General Information

---

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

-

1.14.2 Major Accident Hazards

-

1.14.3 Air Pollution

-

1.15 Additional Remarks

-

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

---

## 2.1 Melting Point

Value: 87 degree C  
Method: other: MPBPWIN Program, version 1.31  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Melting Point: 75.00 deg C (Adapted Joback Method)  
Melting Point: 146.94 deg C (Gold and Ogle Method)  
Mean Melt Pt : 110.97 deg C (Joback; Gold,Ogle Methods)  
Selected MP: 86.99 deg C (Weighted Value)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
27-JUN-2001 (1)

Value: < -70 degree C  
Source: Bayer AG Leverkusen  
12-AUG-1992 (2)

## 2.2 Boiling Point

Value: 446.3 degree C at 1013 hPa  
Method: other: MPBPWIN Program, version 1.31  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Boiling Point: 446.31 deg C (Adapted Stein and Brown Method)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
22-OCT-2001 (1)

Value: ca. 210 degree C at 5 hPa  
Source: Bayer AG Leverkusen  
12-AUG-1992 (2)

## 2.3 Density

Type: density  
Value: .92 g/cm3 at 20 degree C  
Source: Bayer AG Leverkusen  
12-AUG-1992 (2)

## 2.3.1 Granulometry

-

2. Physico-chemical Data

---

## 2.4 Vapour Pressure

Value: .000000205 hPa at 25 degree C  
 Method: other (calculated): MPBPWIN Program, version 1.31  
 Year: 1999  
 GLP: no  
 Testsubstance: other TS: molecular structure  
 Result: Vapor Pressure Estimations (25 deg C):  
       (Using BP: 446.31 deg C (estimated))  
       (Using MP: 86.99 deg C (estimated))  
       VP: 1.17E-008 mm Hg (Antoine Method)  
       VP: 1.54E-007 mm Hg (Modified Grain Method)  
       VP: 3.11E-007 mm Hg (Mackay Method)  
       Selected VP: 1.54E-007 mm Hg (Modified Grain Method)  
 Reliability: (2) valid with restrictions  
               Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (1)

Value: < .01 hPa at 20 degree C  
 Source: Bayer AG Leverkusen  
 12-AUG-1992 (2)

## 2.5 Partition Coefficient

log Pow: 4.2  
 Method: other (measured): according to Saeger et al. (1979)  
 Year: 1979  
 GLP: no data  
 Testsubstance: other TS: tris(2-ethylhexyl)phosphate; obtained from FMC Corporation; purity > 90%  
 Result: octanol/water partition coefficient = 16,800  
 Reliability: (2) valid with restrictions  
               Meets generally accepted scientific standards, well documented  
               and acceptable for assessment  
 Flag: Critical study for SIDS endpoint  
 22-OCT-2001 (3)

log Pow: 4.1  
 Method:  
 Year:  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (4)

log Pow: .7  
 Method: other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989.  
               Daylight, Chemical Information Systems, Claremont, CA 91711,  
               USA  
 Year:  
 Source: Bayer AG Leverkusen  
 12-AUG-1992 (5)

## 2. Physico-chemical Data

---

log Pow: .8  
 Method:  
 Year:  
 Remark: experimentally determined  
 Source: Bayer AG Leverkusen  
 21-SEP-1992 (6)

log Pow: 9.491  
 Method: other (calculated): KOWWIN Program, version 1.65  
 Year: 1999  
 GLP: no  
 Testsubstance: other TS: molecular structure  
 16-OCT-2001 (1)

## 2.6.1 Water Solubility

Value: 2 mg/l  
 Method: other  
 Source: Bayer AG Leverkusen  
 Reliability: (2) valid with restrictions  
 Meets generally accepted scientific standards, well documented  
 and acceptable for assessment  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (7)

Value: .00001 mg/l at 25 degree C  
 Method: other: WSKOW Program, version 1.36  
 Year: 1999  
 GLP: no  
 Testsubstance: other TS: molecular structure  
 Reliability: (2) valid with restrictions  
 Accepted calculation method  
 16-OCT-2001 (1)

Value: < .1 g/l at 20 degree C  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (2)

Value: 1000 other: ppm  
 Method: other: according to Saeger et al. (1979)  
 GLP: no data  
 Testsubstance: other TS: tris(2-ethylhexyl)phosphate; obtained from FMC  
 Corporation; purity > 90%  
 Remark: The true solubility of TEHP is probably less than 1000 ppm,  
 The compound turned cloudy when shaken with water, suggesting  
 the formation of an emulsion or a decomposition product.  
 22-OCT-2001 (3)

## 2.6.2 Surface Tension

-

2. Physico-chemical Data

---

## 2.7 Flash Point

Value: > 170 degree C  
Type: other  
Method: other: DIN 51376  
Year:  
Source: Bayer AG Leverkusen  
12-AUG-1992

(2)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Additional Remarks

-

## 3. Environmental Fate and Pathways

## 3.1.1 Photodegradation

Type: air  
INDIRECT PHOTOLYSIS  
Sensitizer: OH  
Conc. of sens.: 1560000 molecule/cm3  
Rate constant: .000000000097 cm3/(molecule \* sec)  
Degradation: 50 % after 1.3 hour(s)  
Method: other (calculated): AOP Program (v1.89)  
Year: 1999 GLP: no  
Test substance: other TS: molecular structure  
Result: ----- SUMMARY (AOP v1.89): HYDROXYL RADICALS -----  
Hydrogen Abstraction = 97.8576 E-12 cm3/molecule-sec  
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec  
  
OVERALL OH Rate Constant = 97.8576 E-12 cm3/molecule-sec  
HALF-LIFE = 0.109 Days (12-hr day; 1.5E6 OH/cm3)  
HALF-LIFE = 1.312 Hrs  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
27-JUN-2001 (1)  
  
Type:  
Method:  
Year: GLP:  
Test substance:  
Result: ca. 80 % degradation by UV-light (1h)  
Source: Bayer AG Leverkusen  
Flag: Critical study for SIDS endpoint  
26-NOV-1992 (4)

## 3.1.2 Stability in Water

Remark: An attempt to make a water solution of Phosphoric acid, 2-ethylhexyl ester demonstrated that the product was obviously water insoluble and prevented a determination of hydrolysis.  
(See IUCLID on CASRN 12645-31-7)

## 3.1.3 Stability in Soil

-

## 3.2 Monitoring Data (Environment)

-

## 3. Environmental Fate and Pathways

## 3.3.1 Transport between Environmental Compartments

Type: fugacity model level III  
Media: other: air - water - soil - sediment  
Air (Level I):  
Water (Level I):  
Soil (Level I):  
Biota (L.II/III):  
Soil (L.II/III):  
Method: other: Level III Fugacity Model  
Year:  
Result:

Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.312	2.62	1000	7.59e-013
Water	10.9	208	1000	5.02e-017
Soil	31.2	208	1000	1.08e-019
Sediment	57.6	832	0	9e-018

Persistence Time: 350 hr  
Reaction Time: 370 hr  
Advection Time: 6.6e+003 hr  
Percent Reacted: 94.7  
Percent Advected: 5.3  
Remark: Default input values of 1000 kg/hr were used for model.  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
16-OCT-2001

(1)

## 3.3.2 Distribution

-

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

Type: aerobic  
Inoculum: predominantly domestic sewage  
Degradation: 0 % after 28 day  
Result: under test conditions no biodegradation observed  
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"  
Year: 1982 GLP: no  
Test substance: other TS  
Remark: related to BOD  
Source: Bayer AG Leverkusen  
Reliability: (1) valid without restriction  
Guideline study  
Flag: Critical study for SIDS endpoint  
22-OCT-2001

(8)

---

Type: aerobic  
Inoculum: activated sludge  
Concentration: 100 mg/l  
Degradation: 0 % after 28 day  
Result: under test conditions no biodegradation observed  
Method:  
Year: GLP:  
Test substance:  
Remark: Method:  
"Biodegradation test of chemical substance by micro-organisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "301C, Ready Biodegradability: Modified MITI Test I" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).  
related to BOD  
sludge conc.: 30 mg/l  
Source: Bayer AG Leverkusen  
Reliability: (1) valid without restriction  
Guideline study  
Flag: Critical study for SIDS endpoint  
22-OCT-2001 (7)

Type: aerobic  
Inoculum: activated sludge, domestic  
Degradation: 20% ±8% after 238 day  
Method: other: SCAS-Test; EEC Directive 79/831 Annex V Part C  
Year: GLP: no data  
Test substance: other TS: tris(2-ethylhexyl)phosphate; obtained from FMC Corporation; purity > 90%  
Test condition: Concentration: 3 mg/l/24 h  
Reliability: (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment  
Flag: Critical study for SIDS endpoint  
22-OCT-2001 (3)

Type: aerobic  
Inoculum: activated sludge  
Degradation: 55 % after 2 day  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
27-JAN-1994 (4)

Type: aerobic  
Inoculum: other: activated sludge, after acclimatization  
Degradation: 60 % after 2 day  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
27-JAN-1994

(4)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)  
Exposure period: 42 day  
Concentration: 2 mg/l  
BCF: 2.4 - 6.5  
Elimination:  
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"  
Year: 1981 GLP:  
Test substance:  
Remark: log Pow: 5.04  
% lipid average: 5.1  
Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).  
Source: Bayer AG Leverkusen  
22-OCT-2001

(7)

Species: Cyprinus carpio (Fish, fresh water)  
Exposure period: 42 day  
Concentration: .2 mg/l  
BCF: 9.2 - 22  
Elimination:  
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"  
Year: 1981 GLP:  
Test substance:  
Remark: log Pow: 5.04  
% lipid average: 5.1  
Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).

tration in Fish" stipulated in the OECD Guidelines for  
Testing of Chemicals (May 12, 1981).  
Source: Bayer AG Leverkusen  
22-OCT-2001 (7)

Species: other  
Exposure period:  
Concentration:  
BCF: 3.16  
Elimination:  
Method: other: BCF Program (v2.13)  
Year: 1999 GLP: no  
Test substance: other TS: molecular structure  
Result: CHEM : Phosphoric acid, tris(2-ethylhexyl) ester  
MOL FOR: C24 H51 O4 P1  
MOL WT : 434.65  
----- Bcfwin v2.12 -----  
Log Kow (estimated) : 9.49  
Log Kow (experimental): not available from database  
Log Kow used by BCF estimates: 9.49  
  
Equation Used to Make BCF estimate:  
Log BCF = -1.37 log Kow + 14.4 + Correction  
  
Correction(s): Value  
Phosphate ester -0.780  
Alkyl chains (8+ -CH2- groups) -1.500  
Minimum Log BCF of 0.50 applied when Log Kow > 7

Estimated Log BCF = 0.500 (BCF = 3.162)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
27-JUN-2001 (1)

### 3.8 Additional Remarks

Remark: Degradation in natural water: 32-73 %  
Source: Bayer AG Leverkusen  
22-OCT-2001 (9)

## AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

Type: static  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
LC0: >= 100  
Method: other: Letale Wirkung beim Zebrabaerbling,  
UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim  
Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h  
Year: 1982 GLP: no  
Test substance:  
Source: Bayer AG Leverkusen  
Reliability: (2) valid with restrictions  
Meets generally accepted scientific standards, well documented  
and acceptable for assessment  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (8)

Type: static  
Species: Oryzias latipes (Fish, fresh water)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: > 500  
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71)  
"Testing methods for industrial waste water"  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
Reliability: (2) valid with restrictions  
Meets generally accepted scientific standards, well documented  
and acceptable for assessment  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (7)

## 4.2 Acute Toxicity to Aquatic Invertebrates

Remark: Since the mono phosphate is expected to be more toxic than the tris-ester, the acute *Daphnia* LC<sub>50</sub> of the tris-ester is expected to be greater than or equal to that of the bis-ester. Data for the mono- and bis-(2-ethyl hexyl) esters demonstrate 48 hr Acute Invertebrate LC<sub>50</sub> to be >42 mg/l. (See IUCLID data sets on CAS#12645-31-7 and 298-07-7)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

Remark: Acute toxicity to algae has been tested for 2-ethyl hexyl phosphate (12645-31-7) and demonstrated an EC<sub>50</sub> of 161-168 mg/l (Table 3). Since the mono phosphate is expected to be more toxic than the tris-ester, the EC<sub>50</sub> of the tris-ester is expected to be greater than or equal to 161 mg/l. (See IUCLID data set on CAS#12645-31-7)

4. Ecotoxicity

---

## 4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic  
Species: activated sludge  
Exposure period: 3 hour(s)  
Unit: mg/l Analytical monitoring: no  
EC50: > 100  
Method: other: see remarks  
Chemosphere 10 (3), 245-261 (1981)  
Year: 1982 GLP: no  
Test substance:  
Remark: direct weight  
Method: E 3002: The Assessment of the Possible Inhibitory  
Effect of Dyestuffs on Aerobic Waste Water Bacteria.  
Experience with a Screening Test. Brown, D.; Hitz, H.R.;  
Schaefer, L.: Chemosphere 10 (3), 245-261 (1981)  
Source: Bayer AG Leverkusen  
28-JAN-1994

(8)

## 4.5 Chronic Toxicity to Aquatic Organisms

## 4.5.1 Chronic Toxicity to Fish

-

## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

## 4.6.1 Toxicity to Soil Dwelling Organisms

-

## 4.6.2 Toxicity to Terrestrial Plants

-

## 4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

-

## 4.8 Biotransformation and Kinetics

-

## 4.9 Additional Remarks

-

5. Toxicity

---

## 5.1 Acute Toxicity

## 5.1.1 Acute Oral Toxicity

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: 46000 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (10)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: > 36800 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (11)

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: ca. 46000 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
16-OCT-2001 (11)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

---

Type: LD0  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: > 10000 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (12)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: 37080 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (13)

### 5.1.2 Acute Inhalation Toxicity

Type: other: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Exposure time: 4 hour(s)  
Value: > .447 mg/l  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
16-OCT-2001 (11)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

Type: other: LD50  
 Species: guinea pig  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Exposure time: 1 hour(s)  
 Value: > .46 mg/l  
 Method:  
   Year: GLP:  
 Test substance:  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (11)

Type: other: LD50  
 Species: rat  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Exposure time:  
 Value: > .45 mg/l  
 Method:  
   Year: GLP:  
 Test substance:  
 Remark: Exposure time: no data  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (10)

Type: other: LD50  
 Species: guinea pig  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Exposure time:  
 Value: 450 mg/l  
 Method:  
   Year: GLP:  
 Test substance:  
 Remark: Exposure time: no data  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (10)

5. Toxicity

---

## 5.1.3 Acute Dermal Toxicity

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: ca. 20000 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
23-JUL-1992 (10)

## 5.1.4 Acute Toxicity, other Routes

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.v.  
Value: > 358 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
23-JUL-1992 (11)

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: other: intratracheal  
Value: > 1811 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
12-AUG-1992 (11)

5. Toxicity

---

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: irritating

EC classificat.:

Method: other: see remarks

Year:

GLP:

Test substance:

Remark: ear, 24 h exposure, dose not known

Source: Bayer AG Leverkusen

12-AUG-1992

(12)

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: irritating

EC classificat.:

Method: other: see remarks

Year:

GLP:

Test substance:

Remark: 250 mg applied to clipped skin on rabbit back, within 24 h  
moderate erythema which persisted for a week.

Source: Bayer AG Leverkusen

12-AUG-1992

(11)

Species: human

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: not irritating

EC classificat.:

Method: other: see remarks

Year:

GLP:

Test substance:

Remark: 24 h exposure time

Source: Bayer AG Leverkusen

12-AUG-1992

(12)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

### 5.2.2 Eye Irritation

Species: rabbit  
Concentration:  
Dose:  
Exposure Time:  
Comment:  
Number of  
Animals:  
Result: not irritating  
EC classificat.:  
Method: other: see remarks  
Year: GLP:  
Test substance:  
Remark: 0.01 to 0.5 ml, up to 0.05 ml slight conjunctivitis,  
from 0.1 to 0.5 ml moderate conjunctivitis, which cleared  
up within 24 h  
Source: Bayer AG Leverkusen  
26-NOV-1992 (11)

### 5.3 Sensitization

-

### 5.4 Repeated Dose Toxicity

Species: rat Sex: male/female  
Strain: other: F33/N  
Route of admin.: gavage  
Exposure period: 13 weeks  
Frequency of  
treatment: 5 d/w  
Post. obs.  
period: no  
Doses: 250, 500, 1000, 2000 or 4000 mg/kg bw  
Control Group: other: yes (corn oil)  
NOAEL: 1000 mg/kg bw  
LOAEL: 2000 mg/kg bw  
Method: other: EPA OTS 798.3300  
Year: GLP: yes  
Test substance: other TS: tris(2-ethylhexyl) phosphate; purity 97-99%  
Result: no compound related deaths, slight-moderate depression of  
weight gain at 2000 or 4000 mg/kg bw, no histopathologic  
effects.  
Reliability: (1) valid without restriction  
GLP Guideline study  
Flag: Critical study for SIDS endpoint  
17-OCT-2001 (14)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

---

Species:	mouse	Sex: male/female
Strain:	B6C3F1	
Route of admin.:	gavage	
Exposure period:	13 weeks	
Frequency of treatment:	5d/w	
Post. obs. period:	no	
Doses:	500, 1000, 2000, 4000 or 8000 mg/kg bw/d	
Control Group:	other: yes (corn oil)	
NOAEL:	2000 mg/kg bw	
LOAEL:	4000 mg/kg bw	
Method:	other: EPA OTS 798.3300	
Year:		GLP: yes
Test substance:	other TS: tris(2-ethylhexyl) phosphate; purity 97-99%	
Result:	No compound related deaths, slight-moderate depression of weight gain at 4000 or 8000 mg/kg bw, inflammatory lesions in gastric mucosa	
Reliability:	(1) valid without restriction GLP Guideline study	
Flag:	Critical study for SIDS endpoint	
22-OCT-2001		(14)
Species:	rat	Sex: no data
Strain:	no data	
Route of admin.:	oral feed	
Exposure period:	30 d	
Frequency of treatment:	daily	
Post. obs. period:	no	
Doses:	110 to 1550 mg/kg bw/d	
Control Group:	no data specified	
NOAEL:	430 mg/kg	
Method:		
Year:		GLP:
Test substance:		
Result:	at 1550 mg/kg weight loss	
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment	
Flag:	Critical study for SIDS endpoint	
17-OCT-2001		(13)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

---

Species: guinea pig Sex: male  
Strain: Hartley  
Route of admin.: inhalation  
Exposure period: 3 months  
Frequency of treatment: 6h/d, 5d/w  
Post. obs. period: no  
Doses: 1.6 and 9.6 mg/m<sup>3</sup>  
Control Group: yes  
NOAEL: 1.6 mg/m<sup>3</sup>  
LOAEL: 9.6 mg/m<sup>3</sup>  
Method:  
Year: GLP:  
Test substance: other TS: purity of substance not known  
Result: at high level significantly increased terminal body weight, no significant alteration in red blood cell and plasma cholinesterase activity, no abnormalities at necropsy, microscopic examination revealed inconsistent and reversible changes of renal parenchyma of the high level group, sections of the spinal cord and sciatic nerve stained to demonstrate the myelin sheaths showed no pathologic alteration.  
Reliability: (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (11)

Species: dog Sex: male/female  
Strain: other: mongrel dogs  
Route of admin.: inhalation  
Exposure period: 3 months  
Frequency of treatment: 6h/d, 5d/w  
Post. obs. period: no  
Doses: 10.8, 26.4 or 85 mg/m<sup>3</sup>  
Control Group: other: yes  
Method:  
Year: GLP:  
Test substance:  
Remark: purity unknown  
Result: no deaths; evaluation of trained behavior: dose-response relationship in the conditioned avoidance response; no alterations in any of the hematological and biochemical parameters, normal increase in body weights, mild chronic inflammatory changes in pulmonary parenchyma.  
Reliability: (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment  
16-OCT-2001 (11)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

Species: monkey Sex: male/female  
 Strain: other: Rhesus  
 Route of admin.: inhalation  
 Exposure period: 3 months  
 Frequency of treatment: 6h/d, 5d/w  
 Post. obs. period: no  
 Doses: 10.8, 26.4 or 85 mg/m3  
 Control Group: other: yes  
 NOAEL: 85  
 Method:  
 Year: GLP:  
 Test substance: other TS: purity of substance not known  
 Result: no deaths, normal weight gain, no alteration of any of the hematological and biochemical parameters, in the evaluation of trained behavior (visual discrimination test) no effects were detected. No histological abnormalities.  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (11)

Species: guinea pig Sex: male/female  
 Strain: Hartley  
 Route of admin.: inhalation  
 Exposure period: 3 months  
 Frequency of treatment: 6h/d, 5d/w, total 60 exposures  
 Post. obs. period: no  
 Doses: 10.8; 26.4 or 85 mg/m3  
 Control Group: yes  
 Method:  
 Year: GLP:  
 Test substance:  
 Result: high mortality in control group and dosed groups because of intercurrent respiratory infection.  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (11)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

Species: rabbit Sex: no data  
 Strain: other: New Zealand  
 Route of admin.: dermal  
 Exposure period: 2 to 4 weeks  
 Frequency of treatment: 5 d/w  
 Post. obs. period: 3 - 17 d  
 Doses: 0.1 ml/animal  
 Control Group: no  
 Method:  
 Year: GLP:  
 Test substance:  
 Result: animals appeared normal and gained weight, no alterations were observed at necropsy. Skin: moderate erythema following the first application, following subsequent applications, the erythema did not increase in intensity, but a gradual increase in the size of the affected zone was observed. After the fifth application desquamation, hemorrhagic areas, thickening of the skin. Microscopic examination: hyperkeratosis, parakeratosis, good recovery.  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (11)

Species: rat Sex: male/female  
 Strain: other: F344/N  
 Route of admin.: gavage  
 Exposure period: 14 d  
 Frequency of treatment: daily  
 Post. obs. period: no  
 Doses: 375, 750, 1500, 3000 or 6000  
 Control Group: other: yes (corn oil)  
 Method:  
 Year: GLP:  
 Test substance:  
 Result: No animals died, reduced weight gain in male at 1500 mg/kg and higher, in female at 3000 or 6000 mg/kg. No compound related effects at necropsy  
 Source: Bayer AG Leverkusen  
 22-OCT-2001 (14)

## 5. Toxicity

---

Species: mouse Sex: male/female  
 Strain: B6C3F1  
 Route of admin.: gavage  
 Exposure period: 14 d  
 Frequency of treatment: daily  
 Post. obs. period: no  
 Doses: 375, 750, 1500, 3000 or 6000 mg/kg bw/d  
 Control Group: other: yes (corn oil)  
 Method:  
 Year: GLP:  
 Test substance:  
 Result: No animals died. No changes in body weight gain, no compound-related effects at necropsy  
 Source: Bayer AG Leverkusen  
 17-OCT-2001 (14)

Species: cat Sex: no data  
 Strain: no data  
 Route of admin.: gavage  
 Exposure period: 28 d  
 Frequency of treatment: daily  
 Post. obs. period: no  
 Doses: 1 ccm/kg bw/d  
 Control Group: no  
 Method:  
 Year: GLP:  
 Test substance:  
 Result: no clinical signs of toxicity, no inhibition of cholinesterase activity in red blood cells.  
 Source: Bayer AG Leverkusen  
 16-OCT-2001 (12)

## 5.5 Genetic Toxicity 'in Vitro'

Type: Ames test  
 System of testing: S. typhimurium TA 98, 100, 1535, 1537  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP:  
 Test substance:  
 Reliability: (2) valid with restrictions  
 Meets generally accepted scientific standards, well documented and acceptable for assessment  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (14)

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

Type:	Mouse lymphoma assay	
System of testing:	L5178Y	
Concentration:		
Cytotoxic Conc.:		
Metabolic activation:	no data	
Result:	negative	
Method:		
Year:		GLP:
Test substance:		
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment	
Flag:	Critical study for SIDS endpoint	
16-OCT-2001		(15) (16) (17) (18)
Type:	other: Chromosomal aberration	
System of testing:	CHO-cells	
Concentration:		
Cytotoxic Conc.:		
Metabolic activation:	with and without	
Result:	negative	
Method:		
Year:		GLP:
Test substance:		
Flag:	Critical study for SIDS endpoint	
16-OCT-2001		(15) (16) (19) (18)
Type:	Sister chromatid exchange assay	
System of testing:	CHO-cells	
Concentration:		
Cytotoxic Conc.:		
Metabolic activation:	with and without	
Result:	negative	
Method:		
Year:		GLP:
Test substance:		
Flag:	Critical study for SIDS endpoint	
16-OCT-2001		(15) (16) (19) (18)

## 5. Toxicity

---

Type: Ames test  
 System of testing: S. typhimurium TA98, 100, 1535, 1537  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP:  
 Test substance:  
 Source: Bayer AG Leverkusen  
 23-JUL-1992 (20)

Type: Ames test  
 System of testing: S. typhimurium  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: no data  
 Result: negative  
 Method:  
 Year: GLP:  
 Test substance:  
 Source: Bayer AG Leverkusen  
 23-JUL-1992 (15) (16) (18)

Type: Ames test  
 System of testing: S. typhimurium TA 98, TA100, TA1535, TA 1537  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with  
 Result: negative  
 Method:  
 Year: GLP:  
 Test substance:  
 Source: Bayer AG Leverkusen  
 23-JUL-1992 (21)

Type: Ames test  
 System of testing: S. typhimurium TA98, TA100, TA1535, TA1537  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP:  
 Test substance:  
 Remark: purity 97.6 %  
 Source: Bayer AG Leverkusen

23-JUL-1992

(22)

## 5.6 Genetic Toxicity 'in Vivo'

-

## 5.7 Carcinogenicity

Species: rat Sex: male/female  
Strain: Fischer 344  
Route of admin.: gavage  
Exposure period: 2 years  
Frequency of treatment: 5 d/w  
Post. obs. period: no  
Doses: male 2000 or 4000 mg/kg bw/d, female 1000 or 2000 mg/kg bw/d  
Result:  
Control Group: other: yes (corn oil)  
Method: EPA OTS 798.3300  
Year: GLP: yes  
Test substance: other TS: tris(2-ethylhexyl)phosphate; Purity 97-98 %  
Result: no clinical signs of toxicity, depression in body weights only in male animals, survival unaffected, incidence of pheochromocytoma of adrenal glands increased with dose, positive trend for increased incidence of thyroid follicular cell hyperplasia in male rats. In female rats no evidence of carcinogenicity, in male rats equivocal evidence of carcinogenicity in the adrenal gland medulla  
Reliability: (1) valid without restriction  
GLP Guideline study

17-OCT-2001 (23) (24) (25) (14)

Species: mouse Sex: male/female  
Strain: B6C3F1  
Route of admin.: gavage  
Exposure period: 2 years  
Frequency of treatment: 5d/w  
Post. obs. period: no  
Doses: 500 or 1000 mg/kg bw  
Result:  
Control Group: other: yes (corn oil)  
Method: EPA OTS 798.3300  
Year: GLP: yes  
Test substance: other TS: tris(2-ethylhexyl)phosphate; Purity 97-98 %  
Result: no clinical signs of toxicity, no depression in body weights, survival unaffected, increased incidence of follicular cell hyperplasias of the thyroid gland in males and females. No evidence of carcinogenicity in male mice, some evidence of carcinogenicity in female mice (hepatocellular carcinoma).  
Reliability: (1) valid without restriction

## 5. Toxicity

Date: 22-OCT-2001

ID: 78-42-2

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17-OCT-2001 GLP Guideline study (23) (24) (25) (14)

Species: rat Sex: male/female  
Strain: Fischer 344  
Route of admin.: gavage  
Exposure period: 24 months  
Frequency of treatment: 5 days/week  
Post. obs. period: none  
Doses: 50, 150, 500 mg/kg/day  
Result: negative  
Control Group: yes, concurrent vehicle  
Method: EPA OTS 798.3300  
Year: GLP: yes  
Test substance: other TS: 2-ETHYLHEXANOL; purity > 99%  
Remark: 2-ethylhexanol is used in the preparation of tris(2-ethylhexyl)phosphate and believed to be the major metabolic product.  
Result: In decedent and surviving male and female rats recieving 2EH, the incidence of basophilic, eosinophilic, and clear cell foci and focal hyperplasia was not different from that in the vehicle controls. There was no increase in the incidence of hepatocellular carcinomas in rats treated with 2EH.  
Reliability: (1) valid without restriction  
GLP Guideline study

17-OCT-2001 (26)

Species: mouse Sex: male/female  
Strain: B6C3F1  
Route of admin.: gavage  
Exposure period: 18 months  
Frequency of treatment: 5 days/week  
Post. obs. period: none  
Doses: 50, 200, 750 mg/kg/day  
Result:  
Control Group: yes, concurrent vehicle  
Method: EPA OTS 798.3300  
Year: GLP: yes  
Test substance: other TS: 2-ETHYLHEXANOL; purity > 99%  
Remark: 2-ethylhexanol is used in the preparation of tris(2-ethylhexyl)phosphate and believed to be the major metabolic product.  
Result: In surviving female mice, there were no eosinophilic foci and no adenomas and a single hyperplastic focus at 200 mg/kg. There appears to be a correlation between the increased incidence of basophilic foci and hepatocellular carcinomas in female mice, however the increases were only significant at 750 mg/kg. The preneoplastic changes in the livers of female mice, while suggestive of weak oncogenicity, are not conclusive.  
Reliability: (1) valid without restriction

17-OCT-2001 GLP Guideline study

(26)

## 5.8 Toxicity to Reproduction

Remark: Adequate reproductive and developmental studies are available for the two similar chemicals (107-66-4 and 126-73-8). These studies indicate an absence of reproductive or developmental effects of these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, no reproductive or developmental effects of tris (2-ethyl hexyl) phosphate (78-42-2) is expected at doses ranging from >225 to 1000 mg/kg. (See IUCLID data sets on CAS#107-66-4 and 126-73-8)

## 5.9 Developmental Toxicity/Teratogenicity

Remark: Adequate reproductive and developmental studies are available for the two similar chemicals (107-66-4 and 126-73-8). These studies indicate an absence of reproductive or developmental effects of these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, no reproductive or developmental effects of tris (2-ethyl hexyl) phosphate (78-42-2) is expected at doses ranging from >225 to 1000 mg/kg. (See IUCLID data sets on CAS#107-66-4 and 126-73-8) and 126-73-8)

## 5.10 Other Relevant Information

Type:

Remark: hen, gavage: 250, 500 or 1000 mg/kg bw, single application: post exposure examination 2 months, no clinical signs of neurotoxicity.  
hen: i.m.: 250, 500 or 1000 mg/kg bw: no clinical signs of toxicity.

Source: Bayer AG Leverkusen

03-JUN-1993

(12)

Type:

Remark: human cells, in vitro: HeLa-Cells, Metabolic Inhibition Test, 24 h inkubation: no acute toxicity

Source: Bayer AG Leverkusen

23-JUL-1992

(27)

Type:

Remark: hen, single oral dose, 500 or 2500 mg/kg bw, 1 high level animal died, the other appeared normal and maintained or gained weight; macroscopic examination revealed no abnormalities, histological no evidence of demyelinating action.

Source: Bayer AG Leverkusen

23-JUL-1992

(11)

## 5. Toxicity

## Type:

Remark: Radiotracer inhalation study with rats: 9 male rats, single head exposure, 20 minutes, aerosol, sacrifice after 5 min, 30 min, 1, 4, 17, 18, 24, 48, or 70 h:analytical concentration 0.72 to 0.91 mg/l, maximum retention in tissue after the first few hours, fecal excretion high.

Source:

23-JUL-1992

Bayer AG Leverkusen

(11)

## Type:

Method: The "Total Diet Study" uses dietary survey information and analysis of individual food items, and assessed daily intakes of a number of age-sex groups.

Remark: The mean daily intake per unit of body weight

age:	(ug/kg bw/day)
6-11 months	0.0015
2 year	0.0051

14-16 (female)	0.0029
14-16 (male)	0.0033
25-30 (female)	0.0039
25-30 (male)	0.0055
60-65 (female)	0.0033
60-65 (male)	0.0037

16-OCT-2001

(28)

## 5.11 Experience with Human Exposure

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6. References

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## 7. Risk Assessment

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### 7.1 End Point Summary

-

### 7.2 Hazard Summary

-

### 7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 126-73-8
CAS No.	126-73-8
EINECS Name	tributyl phosphate
EINECS No.	204-800-2
TSCA Name	Phosphoric acid tributyl ester
Molecular Formula	C12H27O4P

Producer Related Part

Company:	
Creation date:	22-JUL-1997

Substance Related Part

Company:	
Creation date:	22-JUL-1997

Memo:	Data for Phosphoric Acid Derivatives Category
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Printing date:	16-APR-2001
Revision date:	
Date of last Update:	06-APR-1999

Number of Pages:	79
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Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

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1.0.1 OECD and Company Information

-

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic  
Physical status: liquid  
Purity: = 100 % w/w  
05-NOV-1997

1.1.0 Details on Template

-

1.1.1 Spectra

-

1.2 Synonyms

Phosphoric acid, tributyl ester  
05-NOV-1997

TBP  
05-NOV-1997

1.3 Impurities

CAS-No:  
EINECS-No:  
EINECS-Name:  
Remark: no impurities above normal regulatory levels (1%, 0.1%)  
12-JAN-1999

1.4 Additives

CAS-No:  
EINECS-No:  
EINECS-Name:  
Remark: no data currently available  
27-JAN-1999

1. General Information

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## 1.5 Quantity

## 1.6.1 Labelling

## 1.6.2 Classification

## 1.7 Use Pattern

Type: type  
Category: Non dispersive use  
26-JAN-1999

Type: use  
Category: Solvents  
12-FEB-1998

Type: use  
Category: other: aircraft hydraulic fluid  
26-JAN-1999

Type: use  
Category: other: plasticizer for cellulose acetate, nitrocellulose and  
chlorinated rubber  
12-FEB-1998

## 1.7.1 Technology Production/Use

-

## 1.8 Occupational Exposure Limit Values

Type of limit: TLV (US)  
Limit value: 2.2 mg/m3  
05-NOV-1997

1. General Information

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1.9 Source of Exposure

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

1.14.2 Major Accident Hazards

1.14.3 Air Pollution

1. General Information

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1.15 Additional Remarks

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

## 2. Physico-chemical Data

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### 2.1 Melting Point

Value: < -70 degree C  
22-JUL-1997 (1)

### 2.2 Boiling Point

Value: 130 degree C at 5 hPa  
22-JUL-1997 (1)

### 2.3 Density

Type: density  
Value: .97 g/cm3 at 20 degree C  
22-JUL-1997 (1)

#### 2.3.1 Granulometry

-

### 2.4 Vapour Pressure

Value: .008 hPa at 20 degree C  
22-JUL-1997 (1)

Value: = .00000347 hPa at 25 degree C  
Remark: Guideline D-63-9 to comply with U.S. EPA TSCA Section 4 for  
tributyl phosphate  
06-OCT-1997 (2)

Value: 1 hPa at 97 degree C  
22-JUL-1997 (3)

Value: 10 hPa at 144 degree C  
22-JUL-1997 (3)

### 2.5 Partition Coefficient

log Pow: 2.5  
Method:  
Year:  
GLP: no data  
Remark: experimentally determined  
26-JAN-1999 (4)

2. Physico-chemical Data

---

log Pow: 3.5  
Method: other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989.  
Daylight, Chemical Information Systems, Claremont, CA 91711,  
USA

Year:  
GLP: no data  
26-JAN-1999 (5)

log Pow: 4  
Method:  
Year:  
GLP: no data  
Remark: experimentally determined  
26-JAN-1999 (6)

## 2.6.1 Water Solubility

Value: .4 g/l at 20 degree C  
22-JUL-1997 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

Value: > 150 degree C  
Type:  
Method: other: DIN 51376  
Year:  
GLP: no data  
26-JAN-1999 (1)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Additional Remarks

-

3. Environmental Fate and Pathways

---

## 3.1.1 Photodegradation

Type: other: degradation by UV-radiation  
INDIRECT PHOTOLYSIS  
Degradation: 85 % after 1 hour(s)  
Method:  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999

(7)

## 3.1.2 Stability in Water

Type: abiotic  
Method:  
Year: GLP:  
Test substance:  
Result: After 30 days, there was no evidence of hydrolytic degradation of 14C-tributyl phosphate in any of the buffered solutions.  
Test condition: The hydrolysis of 14C-tributyl phosphate was studied in aqueous buffered solutions of pH 5, 7, and 9 at a nominal concentration of 10.0 ppm. The test was conducted in the dark at 25 degrees C for 30 days.  
29-SEP-1997

(8)

Type:  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: stable in the range pH 3 - 11  
26-JAN-1999

## 3.1.3 Stability in Soil

Type: laboratory Radiolabel: yes  
Concentration:  
Soil temp.: 25 degree C  
Cation exch. capac.  
Microbial biomass:  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: The adsorption/desorption properties of 14C-tributyl phosphate (9B-125, PL89-289, radiopurity 98%) were studied in three different soil types (silt loam, clay loam, sandy loam) at 25 degrees C. The adsorption of TBP reached an equilibrium after 48 hours in all soils using a 0.01M Ca(NO3)2 solution: soil ratio of 5:1. Definitive mean measured test concentrations ranged from 0.516 to 0.101 (0.516, 0.387, 0.300, 0.205 and 0.101) ug/mL. The mean 14C-material balances for all definitive test concentrations

## 3. Environmental Fate and Pathways

with silt loam, clay loam and sandy loam were 95.8%, 101% and 97.7%, respectively. The Freundlich constants ( $K_d$ ) for silt loam, clay loam and sandy loam were 5.84, 7.72, and 3.02, respectively. The adsorption constants as a function of carbon ( $K_{oc}$ ) were 1460, 1188 and 378 for silt loam, clay loam and sandy loam, respectively. The  $K_{oc}$  values indicate that TBP has low mobility in silty loam and clay loam soil types with a medium mobility in sandy loam types.

26-JAN-1999

(9)

## 3.2 Monitoring Data (Environment)

Type of

measurement:

Medium:

air

Method:

Concentration

Remark:

Japan (industrial area): 3.1 - 41.4 ng/m<sup>3</sup>  
( non-industrial): < 10 ng/m<sup>3</sup>

22-JUL-1997

(10)

Type of

measurement:

Medium:

surface water

Method:

Concentration

Remark:

place	concentration (ng/l)	number of measurements proof analyzed	Year
Rhein	max. 3800		1990
Ruhr	600		1990
Emscher	3900		1990
Lippe	800		1990
Wupper	600		1989
Sieg	100		1984
Zuericher See	54 - 82	2	1973
Norwegen			
(River Nitaiva)	100 - 900	3	1979
Japan (Dogo Plein, Ozu Basin area)	ND - 187	4	1974
Japan	20 - 710	16	1975
Japan	6 - 580	39	1977
Japan (Osaka)	20 - 4500	12	1976
Japan (Tokyo)	60 - 2100	12	1978
Japan (Kitakyushu City)	5 - 36	8	1980
Japan (Niigata City)	140	1	1982

25-SEP-1997

(10)

## 3. Environmental Fate and Pathways

Type of  
measurement:

Medium: sediment

Method:

Concentration

Remark:	place	concentration ug/kg	number of measurement proof analyzed		year
	Japan	1.0 - 350	34	100	1975
	Japan	1.9 - 240	48	117	1977
	Japan (Tokyo) river	0.9 - 7.7	13	15	1978
	sea	1.7 - 2.6	3	3	1978
	Japan (Kitakyushu City)	NN**	0	6	1980

22-JUL-1997

(10)

Type of  
measurement:

Medium: biota

Method:

Concentration

Remark:	Fish	: 1.1 - 26 ug/kg
	Crustacea	: 10 - 20 ug/kg
	Birds	: 20 - 250 ug/kg

22-JUL-1997

(10)

## 3.3.1 Transport between Environmental Compartments

Type: adsorption

Media: soil - air

Air (Level I):

Water (Level I):

Soil (Level I):

Biota (L.II/III):

Soil (L.II/III):

Method:

Year:

Remark:	coefficient Koc	1460
	Koc	1188
	Koc	378

22-JUL-1997

(10)

## 3. Environmental Fate and Pathways

## 3.3.2 Distribution

Media:

Method: Calculation according Mackay, Level I

Year:

Remark: air 11 %  
 water 58 %  
 soil 16 %  
 sediment 15 %

22-JUL-1997

(10)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

Type: aerobic

Inoculum: predominantly domestic sewage

Concentration: 100 mg/l

Degradation: 77 % after 28 day

Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"

Year: 1985

GLP: no

Test substance: no data

Remark: related to O<sub>2</sub>-demand

26-JAN-1999

(3)

Type: aerobic

Inoculum: predominantly domestic sewage

Concentration: 3.68 mg/l

Degradation: 92 % after 28 day

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"

Year: 1985

GLP: no

Test substance: no data

Remark: related to BOD

26-JAN-1999

(3)

Type: aerobic

Inoculum: predominantly domestic sewage

Concentration: 20 mg/l related to DOC (Dissolved Organic Carbon)

Degradation: 89 % after 28 day

Method: OECD Guide-line 301 E "Ready biodegradability: Modified OECD Screening Test"

Year: 1985

GLP: no

Test substance: no data

Remark: Primary degradation by activated sludge

96 % 13 w (3 mg/l/24 h)

56 % +/- 21 % 21 w (13 mg/l/24 h)

No difference between biological and chemical degradation.

26-JAN-1999

(6)

### 3. Environmental Fate and Pathways

Date: 16-APR-2001

ID: 126-73-8

Type: aerobic  
 Inoculum: activated sludge, domestic, adapted  
 Concentration: .2 mg/l related to Test substance  
 Degradation: = 91 % after 28 day  
 Method: other: Method similar to OECD 301B  
 Year: GLP: no  
 Test substance: no data  
 Remark: Biodegradation variable; ranged from 3% of theoretical to 91% of theoretical amount of carbon dioxide evolved in 28 days

26-JAN-1999 (11)

Type: aerobic  
 Inoculum: activated sludge  
 Concentration: 30 mg/l related to Test substance  
 Degradation: = 0 - 40 % after 14 day  
 Method: other: see remarks  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Method: "Biodegradation test of chemical substance by organisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "302C, Inherent Biodegradability: Modified MITI Test II" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).  
 sludge conc: 100 mg/l related to BOD

26-JAN-1999 (12)

Type: aerobic  
 Inoculum: activated sludge, domestic, adapted  
 Concentration: 3 mg/l related to Test substance  
 Degradation: > 96 % after 24 hour(s)  
 Method: other: Method similar to OECD 302-A  
 Year: GLP: no  
 Test substance: no data  
 Remark: Biodegradation at 13 mg/L was 56% as loss of parent material

23-SEP-1997 (13)

Type: aerobic  
 Inoculum: activated sludge, domestic, adapted  
 Concentration: related to Test substance  
 Degradation: = 50 % after 5 day  
 Result: other  
 Method: other: River Die-away; Test material spiked into river water and time to 50% degradation determined  
 Year: GLP: no

Test substance: no data  
 25-SEP-1997 (14)

### 3. Environmental Fate and Pathways

---

Type: aerobic  
Inoculum: activated sludge  
Degradation: ca. 30 % after 2 day  
Method:

Year: GLP: no data  
Test substance: no data  
Remark: no details  
26-JAN-1999 (7)

Type: aerobic  
Inoculum: activated sludge  
Degradation: ca. 100 % after 2 day  
Method:

Year: GLP: no data  
Test substance: no data  
Remark: acclimatization  
no details  
26-JAN-1999 (7)

#### 3.6 BOD5, COD or BOD5/COD Ratio

-

#### 3.7 Bioaccumulation

Species: Carassius auratus (Fish, fresh water)  
Exposure period:  
Concentration:  
BCF: 6 - 11  
Elimination:  
Method: OECD Guide-line 305 D "Bioaccumulation: Static Fish Test"  
Year: GLP: no data  
Test substance: no data  
Remark: Carassius auratus: 0.8-2.8 g  
Concentration: 1.7-3.5 mg/l  
26-JAN-1999 (15)

Species: Cyprinus carpio (Fish, fresh water)  
Exposure period:  
Concentration: 60 µg/l  
BCF: 5.5 - 10  
Elimination:  
Method: other: see remarks  
Year: GLP: no data  
Test substance: no data  
Remark: Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).  
26-JAN-1999 (16)

## 3. Environmental Fate and Pathways

Species: Cyprinus carpio (Fish, fresh water)  
 Exposure period:  
 Concentration: 6 µg/l  
 BCF: 6.9 - 20  
 Elimination:  
 Method: other: see remarks  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).  
 26-JAN-1999 (16)

Species: Oryzias latipes (Fish, fresh water)  
 Exposure period:  
 Concentration:  
 BCF: 11 - 49  
 Elimination:  
 Method: OECD Guide-line 305 D "Bioaccumulation: Static Fish Test"  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Concentration: 0.06-4.0 mg/l  
 26-JAN-1999 (17)

Species: Oryzias latipes (Fish, fresh water)  
 Exposure period:  
 Concentration:  
 BCF: 30 - 35  
 Elimination:  
 Method: OECD Guide-line 305 D "Bioaccumulation: Static Fish Test"  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Oryzias latipes: 0.1-0.2 g  
 Concentration: 2-4 mg/l  
 26-JAN-1999 (15)

Species: Oryzias latipes (Fish, fresh water)  
 Exposure period:  
 Concentration:  
 BCF: 16 - 27  
 Elimination:  
 Method: OECD Guide-line 305 E "Bioaccumulation: Flow-through Fish Test"  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Concentration: 0.1-0.84 mg/l  
 26-JAN-1999 (10)

3.8 Additional Remarks

Remark: Degradation by bacteria (*Pseudomonas diminuta*) isolated  
from river water and adapted for two months  
> 50 % after 2 h  
100 % after 43 h  
(Concentration: 2 mg/l, temperature: 40 degree C)

22-JUL-1997

(18)

## AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

Type: flow through  
Species: Oncorhynchus mykiss (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC0: 4.3  
LC50: 13  
LC100: 19  
Method: other: Methods for Acute Toxicity Tests with Fish,  
Macroinvertebrates and Amphibians. EPA, Ecological Research  
Series EPA-660/3-75-009, April 1975, U.S. EPA-TSCA, 40 CFR,  
Part 797 (1985)  
Year: GLP: no data  
Test substance: no data  
Test condition: Temperature: 12 degree C  
26-JAN-1999 (19)

Type: semistatic  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 10 day  
Unit: mg/l Analytical monitoring: no  
\* : 13.5  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: \* threshold concentration  
Embryo-larval toxicity test  
Nominal concentration; without feeding;  
25 degree C  
26-JAN-1999 (20)

Type: semistatic  
Species: Salmo gairdneri (Fish, estuary, fresh water)  
Exposure period: 50 day  
Unit: mg/l Analytical monitoring: no  
\* : 8.3  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: \* threshold concentration  
Embryo-larval toxicity test  
Nominal concentration; without feeding;  
8 degree C  
26-JAN-1999 (20)

---

Type: static  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 144 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 11.4  
Method: other: ISO 1975  
Year: GLP: no data  
Test substance: no data  
Test condition: pH 7.3 - 8.5  
Temperature: 25 degree C  
26-JAN-1999 (20)

Type: static  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
LC0: 10  
LC100: 14  
Method: other: Letale Wirkung beim Zebrabaerbling,  
UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim  
Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h  
Year: 1985 GLP: no  
Test substance: no data  
Remark: geom. mean: 11.8  
Nominal concentration  
26-JAN-1999 (3)

Type: static  
Species: Carassius auratus (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: yes  
LC50: 8.8  
Method:  
Year: GLP: no data  
Test substance: no data  
Test condition: Temperature: 25 degree C  
26-JAN-1999 (15)

Type: static  
Species: Leuciscus idus (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
LC0: 5.8  
LC50: 7.6  
LC100: 8.7  
Method: other: DEV, L 15 (1976)  
Year: GLP: no  
Test substance: no data  
26-JAN-1999 (21)

## 4. Ecotoxicity

Date: 16-APR-2001  
ID: 126-73-8

Type: static  
Species: Oncorhynchus mykiss (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
NOEC: = 4.9  
LC50: = 11  
Method: other: method similar to OECD 203  
Year: GLP: yes  
Test substance: no data  
Remark: 24 hour LC50 = 13 mg/l; 48 hour LC50 = 11 mg/l.  
23-SEP-1997 (22)

Type: static  
Species: Oncorhynchus mykiss (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: yes  
LC50: 11.5 - 13.5  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: Nominal concentration  
measured concentration: 5 - 9 mg/l,  
no details about control;  
only 4 fish for each concentration.  
Test condition: 15 degree C  
26-JAN-1999 (23)

Type: static  
Species: Oryzias latipes (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: yes  
LC50: 9.6  
Method:  
Year: GLP: no data  
Test substance: no data  
Test condition: Temperature: 25 degree C  
26-JAN-1999 (15)

Type: static  
Species: Pimephales promelas (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
NOEC: = 3.2  
LC50: = 6.4  
Method: other: method similar to OECD 203  
Year: GLP: yes  
Test substance: no data  
Remark: 24 hour LC50=10 mg/l; 48 hour LC50=9.6 mg/l  
26-JAN-1999 (24)

## 4. Ecotoxicity

Date: 16-APR-2001

ID: 126-73-8

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Type: static  
Species: Salmo gairdneri (Fish, estuary, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 4.2  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: Nominal concentration  
Test condition: 20 degree C  
26-JAN-1999 (25)

Type: static  
Species: Salmo gairdneri (Fish, estuary, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 8.2  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: Nominal concentration  
Test condition: 15 degree C  
26-JAN-1999 (25)

Type: static  
Species: Salmo gairdneri (Fish, estuary, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 11.8  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: Nominal concentration  
Test condition: 10 degree C  
26-JAN-1999 (25)

Type: static  
Species: Oryzias latipes (Fish, fresh water)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 4.5  
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (26)

---

Type:  
Species: Oryzias latipes (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 4.5  
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (26)

Type:  
Species: Oryzias latipes (Fish, fresh water)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 14.2  
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71)  
"Testing methods for industrial waste water"  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (16)

Type:  
Species: Oryzias latipes (Fish, fresh water)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 18  
Method:  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (27)

Type:  
Species: Pimephales promelas (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: yes  
LC50: 8.18  
EC50 : 7.79  
Method:  
Year: GLP: no data  
Test substance: as prescribed by 1.1 - 1.4  
Remark: gas-liquid chromatography  
Test condition: Temperature: 25.9 degree C  
26-JAN-1999 (28)

#### 4. Ecotoxicity

Date: 16-APR-2001  
ID: 126-73-8

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Type:  
Species: Pimephales promelas (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: yes  
LC50: 11  
EC50 : 6.56  
Method:  
Year: GLP: no data  
Test substance: as prescribed by 1.1 - 1.4  
Remark: gas-liquid chromatography  
Test condition: Temperature: 26.7 degree C  
26-JAN-1999 (28)

#### 4.2 Acute Toxicity to Aquatic Invertebrates

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 4.2  
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (26)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring: no  
EC0: 2.5  
EC50: 5.8  
EC100: 20  
Method: other: Daphnien-Schwimmunfaehigkeits-Test, UBA-Verfahrensvorschlag Mai 1984, Bestimmung der Schwimmunfaehigkeit beim Wasserfloh Daphnia magna, EC0, EC50, EC100 24h, statisches System  
Year: 1985 GLP: no  
Test substance: no data  
26-JAN-1999 (3)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 12.8  
Method: other: ISO (1975)  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (29)

## 4. Ecotoxicity

Date: 16-APR-2001

ID: 126-73-8

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Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 3.65  
Method: other: ISO (1975)  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (29)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 72 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 2.1  
Method: other: ISO (1975)  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (29)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 14 day  
Unit: mg/l Analytical monitoring:  
NOEC: 3.1  
Method: other: OECD Guide-line 202, Daphnia sp., acute immobilization and reproduction test  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (26)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring: no  
NOEC: = 1.8  
EC50: = 9  
Method: other: method similar to OECD 202  
Year: GLP: yes  
Test substance: no data  
Remark: 24 hour EC50 = 23 mg/l.  
26-JAN-1999 (30)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC0: 5  
EC50: 30  
EC100: 41  
Method: other: static  
Year: GLP: no  
Test substance: no data  
26-JAN-1999 (31)

## 4. Ecotoxicity

Date: 16-APR-2001  
ID: 126-73-8

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Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC0: 7  
EC50: 33  
EC100: 58  
Method: other: static  
Year: GLP: no  
Test substance: no data  
Remark: Nominal concentration  
Test condition: Temperature: 20 - 22 degree C  
26-JAN-1999 (32)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 6 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 52  
Method:  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (33)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC0: 9.3  
EC50: 35  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: Nominal concentration  
26-JAN-1999 (34)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 35  
Method:  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (33)

## 4. Ecotoxicity

Date: 16-APR-2001

ID: 126-73-8

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Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring: yes  
NOEC: = .75  
EC50: = 2.6  
Method:  
Year: 1990 GLP: yes  
Test substance: no data  
26-JAN-1999 (35)

Type:  
Species: Daphnia pulex (Crustacea)  
Exposure period: 6 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 93  
Method:  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (33)

Type:  
Species: Daphnia pulex (Crustacea)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 68  
Method:  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (33)

Type:  
Species: other: Gammarus pseudolimnaeus  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
NOEC: .52  
LC50 : 1.7  
Method: other: see remarks  
Year: GLP: no data  
Test substance: no data  
Remark: Methods for Acute Toxicity Tests with Fish,  
Macroinvertebrates and Amphibians, 795.120 of the Federal  
Register Guideline "Gammarid Acute Toxicity Test" and  
Standard Methods for Examination of Water and Wastewater  
(flow-through bioassay)  
Length: 2 - 3 mm  
Mortality and Immobilisation  
Nominal concentration  
26-JAN-1999 (36)

#### 4. Ecotoxicity

Date: 16-APR-2001

ID: 126-73-8

Type:  
 Species: other: *Hyalella azteca*  
 Exposure period: 96 hour(s)  
 Unit: mg/l Analytical monitoring:  
 NOEC: < 1.9  
 LC50 : 2.4  
 Method: other: see remarks  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Length: 1 - 2 mm  
 Nominal concentration  
 Methods for Acute Toxicity Tests with Fish,  
 Macroinvertebrates and Amphibians, 795.120 of the Federal  
 Register Guideline "Gammarid Acute Toxicity Test" and  
 Standard Methods for Examination of Water and Wastewater  
 (flow-through bioassay).

26-JAN-1999 (37)

#### 4.3 Toxicity to Aquatic Plants e.g. Algae

Species: *Chlorella vulgaris* (Algae)  
 Endpoint:  
 Exposure period: 7 day  
 Unit: mg/l Analytical monitoring:  
 EC50: 5  
 Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"  
 Year: GLP: no data  
 Test substance: no data  
 26-JAN-1999

(26)

Species: *Microcystis aeruginosa* (Algae, blue, cyanobacteria)  
 Endpoint:  
 Exposure period: 8 day  
 Unit: mg/l Analytical monitoring: no  
 TT : 4.1  
 Method: other: cell multiplication inhibition test  
 Year: GLP: no  
 Test substance: no data  
 Test condition: Temperature: 27 degree C  
 26-JAN-1999

(38)

Species: *Scenedesmus quadricauda* (Algae)  
 Endpoint:  
 Exposure period: 8 day  
 Unit: mg/l Analytical monitoring: no  
 TT : 3.2  
 Method: other: cell multiplication inhibition test  
 Year: GLP: no  
 Test substance: no data  
 Test condition: Temperature: 25 degree C  
 26-JAN-1999

(39)

---

Species: Scenedesmus subspicatus (Algae)  
Endpoint:  
Exposure period: 72 hour(s)  
Unit: mg/l Analytical monitoring:  
Method: other: Scenedesmus-Zellvermehrungs-Hemmtest, DIN 38412 Teil 9, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Gruenalgen  
Year: GLP: no data  
Test substance: no data  
Remark: EC10 (biomass): 0.37; EC50 (biomass): 1.1  
EC10 (growth rate): 0.92; EC50 (growth rate): 2.8  
26-JAN-1999 (40)

Species: Selenastrum capricornutum (Algae)  
Endpoint:  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
NOEC: 2.2  
EC50: 4.4  
Method: other: static (ABC Protocol 8004-PMN)  
Year: GLP: no data  
Test substance: no data  
Test condition: Temperature: 24 degree C  
26-JAN-1999 (41)

Species: other algae: Chlorella emersonii  
Endpoint:  
Exposure period: 2 day  
Unit: mg/l Analytical monitoring:  
EC50: 5 - 10  
Method:  
Year: GLP: no data  
Test substance: no data  
Test condition: Temperature: 25 degree C  
26-JAN-1999 (25)

Species: other aquatic plant: Phytoplankton (13 species)  
Endpoint: growth rate  
Exposure period: 14 day  
Unit: mg/l Analytical monitoring:  
EC100 : 50  
Method: other: Microtiter-Plates, visual evaluation  
Year: GLP: no data  
Test substance: no data  
Remark: LOEC 5 mg/l  
26-JAN-1999 (42)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic  
Species: activated sludge  
Exposure period: 3 hour(s)  
Unit: mg/l Analytical monitoring: no  
EC50: 300  
Method: ISO 8192 "Test for inhibition of oxygen consumption by  
activated sludge"  
Year: 1985 GLP: no  
Test substance: no data  
Remark: direct weight  
26-JAN-1999 (3)

Type: aquatic  
Species: activated sludge of a predominantly domestic sewage  
Exposure period: 3 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 100  
Method: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition  
Test"  
Year: GLP: no data  
Test substance: no data  
26-JAN-1999 (27)

Type: aquatic  
Species: Pseudomonas putida (Bacteria)  
Exposure period: 16 hour(s)  
Unit: mg/l Analytical monitoring: no  
TT : > 100  
Method:  
Year: GLP: no  
Test substance: no data  
Test condition: Temperature: 25 degree C  
26-JAN-1999 (43)

## 4. Ecotoxicity

## 4.5 Chronic Toxicity to Aquatic Organisms

## 4.5.1 Chronic Toxicity to Fish

Species: Oncorhynchus mykiss (Fish, fresh water)  
 Endpoint: other: time to swim-up stage; survival, length and weight  
 Exposure period: 95 day  
 Unit: mg/l Analytical monitoring: yes  
 NOEC: = .82  
 LOEC: = 1.7  
 MATC : = 1.2  
 Method: other: U.S. EPA. 1987. Fish Early Life Stage Toxicity Test  
 (Amended. Federal Register, Vol. 52, No. 97/Wed., May 20,  
 1987; Part 797.1600 Amended: 19064-19066  
 Year: 1991 GLP: yes  
 Test substance: no data  
 Remark: Results based on measured concentrations.  
 26-JAN-1999 (44)

## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)  
 Endpoint: other: EC50: based on immobilization; 21-Day LOEC: based on  
 length, days to first brood and Y/D/D  
 Exposure period: 21 day  
 Unit: mg/l Analytical monitoring: yes  
 NOEC: = .87  
 LOEC: = 2.1  
 EC50: > 2.1  
 MATC : = 1.35  
 Method:  
 Year: 1991 GLP: yes  
 Test substance: no data  
 26-JAN-1999 (45)

Species: Daphnia magna (Crustacea)  
 Endpoint:  
 Exposure period: 21 day  
 Unit: mg/l Analytical monitoring:  
 NOEC: 1.3  
 Method: other: "Verlaengerter Toxizitaetstest bei Daphnia magna  
 (Bestimmung der NOEC fuer Reproduktionsrate, Mortalitaet und  
 den Zeitpunkt des ersten Auftretens von Nachkommen; 21 d)  
 Stand: 01.01.1984"  
 Year: GLP: no data  
 Test substance: no data  
 Remark: Nominal concentration  
 measured value: 1.0 mg/l  
 26-JAN-1999 (34)

## TERRESTRIAL ORGANISMS

## 4.6.1 Toxicity to Soil Dwelling Organisms

Type:

Species:

Endpoint:

Exposure period:

Unit:

Method:

Year:

GLP:

Test substance:

Remark: No mortality was observed among two-spotted spider mites  
(Tetranychus urticae) fed TBP at a concentration of 2 g/kg.

06-OCT-1997

(46)

## 4.6.2 Toxicity to Terrestrial Plants

Species:

Endpoint:

Expos. period:

Unit:

Method:

Year:

GLP: no data

Test substance: no data

Remark: TBP is used as a constituent of cotton defoliants,  
producing leaf scorching, and is associated with an  
increase in the rate of leaf drying.

27-JAN-1999

(46)

Species:

Endpoint:

Expos. period:

Unit:

Method:

Year:

GLP: no data

Test substance: no data

Remark: TBP increases the drying rate of lucerne, resulting  
in excessive leaf loss.

27-JAN-1999

(46)

Species:

Endpoint:

Expos. period:

Unit:

Method:

Year:

GLP: no data

Test substance: no data

Remark: TBP applied by spraying as an emulsion (at a rate  
equivalent to 0.25 % of freshly harvested leaf/weight)  
doubled the drying rate of ryegrass leaves. Leaf respir-  
ation stopped and did not resume in the subsequent 4 days.

27-JAN-1999

(46)

Species:  
Endpoint:  
Expos. period:  
Unit:  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: TBP has been shown to damage the leaf surface and help  
herbicides penetrate bean leaves.  
27-JAN-1999 (46)

Species:  
Endpoint:  
Expos. period:  
Unit:  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: There is no information on the effects of TBP on non-  
target plants, even at concentrations designed to produce  
desiccation of crop plants.  
27-JAN-1999 (46)

#### 4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

-

#### 4.7 Biological Effects Monitoring

-

#### 4.8 Biotransformation and Kinetics

-

#### 4.9 Additional Remarks

Remark: TT 14 mg/l (Entosiphon sulcatum, 3 d)  
TT 21 mg/l (Uronema Parduczi, 20 h)  
TT 42 mg/l (Chilomonas parameaecium, 2 d)  
Source: Bayer AG Leverkusen 1  
22-JUL-1997 (47)

Remark: EC50 20 mg/l (Tetrahymena pyriformis, 24 h)  
22-JUL-1997 (27)

5. Toxicity

---

## 5.1 Acute Toxicity

## 5.1.1 Acute Oral Toxicity

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1552 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: = 1.6 ml/kg  
27-JAN-1999 (48)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: 1600 - 3200 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (49)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 3000 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (49) (50)

## 5. Toxicity

Date: 16-APR-2001  
ID: 126-73-8

---

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1400 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (51)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 3350 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (52)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1390 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: male rats  
20-JAN-1999 (53)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1530 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: female rats  
20-JAN-1999 (54)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

---

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 11265 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (55)

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: < 20000 mg/kg bw  
Method:  
Year: GLP: no  
Test substance: no data  
20-JAN-1999 (56)

Type: LD50  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: 400 - 800 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (49)

Type: LD50  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1189 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (52)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

---

Type: LD50  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1240 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: male mice  
20-JAN-1999 (54)

Type: LD50  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 900 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: female mice  
20-JAN-1999 (54)

Type: LD50  
Species: hen  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1500 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (57)

Type: LD50  
Species: hen  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 1800 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (51)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

Type: LD50  
 Species: hen  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Value: = 1500 mg/kg bw  
 Method:  
   Year: GLP: no data  
 Test substance: no data  
 27-JAN-1999 (58)

### 5.1.2 Acute Inhalation Toxicity

Type: LC0  
 Species: rat  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Exposure time: 6 hour(s)  
 Value: = 1.5 mg/l  
 Method:  
   Year: GLP: no data  
 Test substance: no data  
 Remark: = 123 ppm  
   mortality: 0/3  
   strong skin and respiratory irritant  
 27-JAN-1999 (59)

Type: LC50  
 Species: rat  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Exposure time: 6 hour(s)  
 Value: > 42 mg/l  
 Method:  
   Year: GLP: no data  
 Test substance: no data  
 Remark: with 3800 ppm (calculated): mortality 1/3, irritation  
   = 42 mg/l 6h  
   with 350 ppm (calculated, = 4 mg/l): irritation, no  
   mortalities (no further data).  
 20-JAN-1999 (49)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

---

Type: LC50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Exposure time: 1 hour(s)  
Value: = 28 mg/l  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (60)

Type: LC50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Exposure time: 4 hour(s)  
Value: > 4.242 mg/l  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: maximum producable concentration = 4.242 mg/l,  
aerosol, analytical value.  
2/5 male animals died, 0/5 female animals died  
test according OECD guideline 403  
27-JAN-1999 (61)

Type: LC50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Exposure time: 1 hour(s)  
Value: < 200 mg/l  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (62) (56)

5. Toxicity

---

Type: LC50  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Exposure time:  
Value: = 1.3 mg/l  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: only calculated value, no experimental study  
20-JAN-1999 (52)

Type: other: LC  
Species: cat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Exposure time: 5 hour(s)  
Value: = 24.51 mg/l  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (63)

## 5.1.3 Acute Dermal Toxicity

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: > 3100 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (51)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

---

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: > 10000 mg/kg bw  
Method:  
Year: GLP: no  
Test substance: no data  
20-JAN-1999 (56) (64)

Type: LD50  
Species: guinea pig  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: 9700 - 19400 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: application of 10 - 20 ml/kg bw  
20-JAN-1999 (49)

### 5.1.4 Acute Toxicity, other Routes

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.p.  
Value: 800 - 1600 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
20-JAN-1999 (49)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

Type: LD50  
 Species: rat  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Route of admin.: i.p.  
 Value: = 251.2 mg/kg bw  
 Method:  
   Year: GLP: no data  
 Test substance: no data  
 20-JAN-1999 (52)

Type: LD50  
 Species: mouse  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Route of admin.: i.p.  
 Value: 100 - 200 mg/kg bw  
 Method:  
   Year: GLP: no data  
 Test substance: no data  
 20-JAN-1999 (49)

Type: LD50  
 Species: mouse  
 Strain:  
 Sex:  
 Number of  
   Animals:  
 Vehicle:  
 Route of admin.: i.p.  
 Value: = 158.5 mg/kg bw  
 Method:  
   Year: GLP: no data  
 Test substance: no data  
 20-JAN-1999 (52)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

---

Type: other: LD  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.p.  
Value: = 1000 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: 1000 or 5000 mg/kg bw were fatal within 1/2 to 4 hours.  
With 500 mg/kg bw coma for 24 hours, than recovery.  
with 50 or 100 mg neither behavioral nor pathological  
changes.  
27-JAN-1999 (23)

Type: other: LD  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: s.c.  
Value: = 3000 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
27-JAN-1999 (63)

Type: other: LD  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.v.  
Value: 80 - 100 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: 80 mg/kg sublethal, 100 mg/kg lethal, no cholinergic  
symptoms  
27-JAN-1999 (65)

## 5. Toxicity

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: slightly irritating

EC classificat.:

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"

Year:

GLP: no data

Test substance: no data

27-JAN-1999

(66)

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: irritating

EC classificat.:

Method: other: see remarks

Year:

GLP: no data

Test substance: no data

Remark:

- concentrated tributyl phosphate:  
 ear, occlusive 24 hours, soaked cotton swab or  
 single painted ear: irritation  
 - 50 % in Lanoline:  
 ear, occlusive, 24 hours: irritation  
 - 10 % in Lanoline:  
 no irritation

27-JAN-1999

(67)

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: highly irritating

EC classificat.:

Method: other: no data

Year:

GLP: no

Test substance: no data

20-JAN-1999

(68) (50)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: slightly irritating

EC classificat.:

Method: other: no data

Year:

GLP: no

Test substance: no data

20-JAN-1999

(62)

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: highly irritating

EC classificat.:

Method: other: see remarks

Year:

GLP: no

Test substance: no data

Remark: single dermal application of 500 mg/animal on intact or  
abraded skin of six rabbits.

20-JAN-1999

(69)

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: irritating

EC classificat.:

Method: other: see remarks

Year:

GLP: no data

Test substance: no data

Remark: the neat liquid or 10 % aqueous solutions applied on three  
to ten occasions to the intact or abraded skin: slight  
hyperaemia, tissue damage (no further data).

27-JAN-1999

(70)

Species: rabbit  
Concentration:

Exposure:  
Exposure Time:  
Number of  
Animals:

PDII:  
Result: highly irritating  
EC classificat.:  
Method: other: exposure period 24 hours, no further data  
Year: GLP: no  
Test substance: no data  
20-JAN-1999

(71)

Species: guinea pig  
Concentration:

Exposure:  
Exposure Time:  
Number of  
Animals:

PDII:  
Result: irritating  
EC classificat.:  
Method: other: see remarks  
Year: GLP: no data  
Test substance: no data  
Remark: skin, 24 hours contact under an impervious covering.  
20-JAN-1999

(49)

Species: guinea pig  
Concentration:

Exposure:  
Exposure Time:  
Number of  
Animals:

PDII:  
Result: highly irritating  
EC classificat.:  
Method: other: see remarks  
Year: GLP: no data  
Test substance: no data  
Remark: covered contact with the neat liquid for 24 hours (no further data).  
A 10 % solution in dimethyl phthalate was slightly irritating when applied to intact skin and moderately irritating when applied to abraded skin, whereas 2 % concentration caused no irritation (no further data).

27-JAN-1999

(72)

Species: human  
Concentration:

Exposure:  
Exposure Time:  
Number of  
Animals:

PDII:

Result: irritating

EC classificat.:

Method: other: see remarks

Year:

GLP: no data

Test substance: no data

Remark: - concentrated tributyl phosphate:  
arm, soaked cotton swab: irritation.  
- 75 % in Lanoline:  
arm, occlusive, 3 hours: irritation.  
- 50 % in Lanoline:  
arm, soaked cotton swab, 24 hours: mild irritation  
- 10 % in Lanoline:  
arm, soaked cotton swab, occlusive, 24 hours: no  
irritation

27-JAN-1999

(67)

Species: rat  
Concentration:

Exposure:  
Exposure Time:  
Number of  
Animals:

PDII:

Result: highly irritating

EC classificat.:

Method: other: see remarks

Year:

GLP: no data

Test substance: no data

Remark: covered contact with the neat liquid for 5 days

27-JAN-1999

(73)

### 5.2.2 Eye Irritation

Species: rabbit  
Concentration:

Dose:  
Exposure Time:  
Comment:  
Number of  
Animals:

Result: slightly irritating

EC classificat.:

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"

Year:

GLP: no data

Test substance: no data

## 5. Toxicity

Date: 16-APR-2001

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(66)

Species: rabbit

Concentration:

Dose:

Exposure Time:

Comment:

Number of

Animals:

Result: irritating

EC classificat.:

Method: other: no data

Year:

GLP: no

Test substance: no data

Remark: eye injury after 24 hour instillation

not irritant if washed out 4 seconds after instillation

20-JAN-1999

(62) (71) (50)

Species: rabbit

Concentration:

Dose:

Exposure Time:

Comment:

Number of

Animals:

Result: slightly irritating

EC classificat.:

Method: other: see remarks

Year:

GLP: no

Test substance: no data

Remark: instillation of 100 mg/animal, observation period min. 7

days

20-JAN-1999

(69)

Species: other: no data

Concentration:

Dose:

Exposure Time:

Comment:

Number of

Animals:

Result: irritating

EC classificat.:

Method: other: no data

Year:

GLP: no data

Test substance: no data

Remark: transient irritation

20-JAN-1999

(49)

## 5.3 Sensitization

Type: Open epicutaneous test  
Species: guinea pig  
Number of Animals:  
Vehicle:  
Result: not sensitizing  
Classification:  
Method: other: test according EPA final test rule 1989, Test standard 40CFR 798.4100  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: once weekly dermal application until a total of 3 applications, 14 day rest period, dermal challenge on a virgin site.

20-JAN-1999 (74)

Type: Patch-Test  
Species: human  
Number of Animals:  
Vehicle:  
Result:  
Classification:  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: 53 volunteers, 15 applications of a formulation, said to contain less than 25 % tributyl phosphate, were made on alternate days. No volunteer gave local reactions 24 hours after the final patch, therefore no evidence of sensitization.

27-JAN-1999 (75)

Type: other: standard test  
Species: guinea pig  
Number of Animals:  
Vehicle:  
Result: sensitizing  
Classification:  
Method: other: standard sensitization test  
Year: GLP: no data  
Test substance: no data  
Remark: positive with 6 out of 15 animals ( no further data ).

20-JAN-1999 (49)

## 5. Toxicity

## 5.4 Repeated Dose Toxicity

Species: rat Sex: no data  
 Strain: no data  
 Route of admin.: inhalation  
 Exposure period: 4 months  
 Frequency of treatment: 5 days/week, 5 hours/day  
 Post. obs. period: 1 months  
 Doses: 5.1 or 13.6 mg/m3  
 Control Group: no data specified  
 Method: GLP: no data  
 Year:  
 Test substance: no data  
 Remark: group size and purity not mentioned  
 Result: in the high concentration decrease of cholinesterase activity to 33 % after 3 months, effects on physiological and biochemical parameters esp. of the liver. The cholinesterase activity returned to normal in the postexposure period. In the low concentration no effect on cholinesterase activity (no further data).

20-JAN-1999

(52)

Species: rat Sex: male/female  
 Strain: Sprague-Dawley  
 Route of admin.: oral feed  
 Exposure period: 13 weeks  
 Frequency of treatment: daily (feeding study)  
 Post. obs. period: no  
 Doses: 8, 40, 200, 1000 or 5000 mg/kg diet (0.6, 3, 15, 75 or 375 mg/kg)  
 Control Group: yes  
 Method: GLP: yes  
 Year:  
 Test substance: as prescribed by 1.1 - 1.4  
 Remark: 15 animals/sex/group  
 purity not known  
 Result: depressed red blood counts and increased prothrombin and thromboplastin times in males (5000 ppm), increased gamma-GT levels and increased absolute and relative liver weights in both sexes at 5000 ppm. Histopathology: transitional cell hyperplasia in the urinary bladders of both sexes at the 5000 ppm level and males at the 1000 ppm level. No microscopic changes in nerve tissues, bone marrow or liver, or remarkable changes in cholinesterase levels were seen.

20-JAN-1999

(76)

## 5. Toxicity

Date: 16-APR-2001

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Species: rat Sex: male  
Strain: Wistar  
Route of admin.: oral feed  
Exposure period: 3 months  
Frequency of treatment: daily (feeding study)  
Post. obs. period: no  
Doses: 500, 2000 or 10000 mg/kg diet (37.5, 150 or 750 mg/kg bw)  
Control Group: yes  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: purity and group size not mentioned  
Result: dose-dependent depression of body weight gain, increments of liver, kidney and testis weight, and decrease in uterus weight, no changes in hematological analysis except an increment on BUN value with high level of TBP (no further data).

20-JAN-1999

(54)

Species: rat Sex: male  
Strain: Wistar  
Route of admin.: oral feed  
Exposure period: 10 weeks  
Frequency of treatment: daily (feeding study)  
Post. obs. period: no  
Doses: 5000 or 10000 mg/kg diet (375 or 750 mg/kg bw)  
Control Group: yes  
Method:  
Year: GLP: no data  
Test substance: other TS: purity > 97 %  
Remark: 10-11 animals/group  
Result: dose dependent decrease of body weight gain, decreased food consumption, decreased absolute weight of brain and kidneys, increase of total protein and cholesterol in the high dose group, increase of urea nitrogen and prolongation of blood coagulation in both treatment groups, decrease of activity of transaminases in both treatment groups, brain cholinesterase activity in the treatment groups was higher than in the control group, no change of cholinesterase activity in liver and serum.

20-JAN-1999

(77)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

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Species: rat Sex: male  
Strain: Wistar  
Route of admin.: oral feed  
Exposure period: 9 weeks  
Frequency of treatment: daily (feeding study)  
Post. obs. period: no  
Doses: 5000 mg/kg diet (375 mg/kg bw)  
Control Group: yes  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: 8 rats in the treatment group, 18 rats in the control group, purity not known  
Result: decreased body weight gain, increased absolute and relative liver weight, unchanged hematologic values, increase of blood urea nitrogen, unchanged serum enzyme activity (transaminases, phosphatase, cholinesterase).  
20-JAN-1999 (78)

Species: rat Sex: male/female  
Strain: Sprague-Dawley  
Route of admin.: gavage  
Exposure period: 2 weeks  
Frequency of treatment: daily  
Post. obs. period: no  
Doses: 0.14 or 0.42 ml/kg bw (136 or 400 mg/kg bw)  
Control Group: yes  
Method:  
Year: GLP: no data  
Test substance: other TS: purity 98.4 %  
Remark: 10 animals/sex/group  
Result: no overt signs of toxicity, decrease of Hb in high dose females, some changes of clinical chemistry parameters, increase of liver weight and liver to body ratio in high-dose groups, decrease of spleen weight in the high-dose female group, no gross morphological changes, one out of four male rats (high-dose group) showed microscopic degenerative changes in seminiferous tubules.  
20-JAN-1999 (79)

## 5. Toxicity

Date: 16-APR-2001

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Species: rat Sex: male/female  
Strain: Sprague-Dawley  
Route of admin.: gavage  
Exposure period: 18 weeks  
Frequency of treatment: 5 days/week  
Post. obs. period: no  
Doses: 0.2 or 0.3-0.35 ml/kg bw (200 or 300-350 mg/kg bw)  
Control Group: yes  
Method: GLP: no data  
Year:  
Test substance: other TS: purity 98.4 %  
Remark: 12 animals/sex/group  
Result: No overt signs of toxicity, decrease of body weight in high-dose males, no changes in hematological and biochemical parameters besides decrease of red blood cell acetylcholin-esterase, in high-dose females increase of liver weight and spleen weight, diffuse urothelial hyperplasia of urinary bladder in both sexes, no testicular changes.

20-JAN-1999

(80)

Species: rat Sex: male/female  
Strain: Sprague-Dawley  
Route of admin.: gavage  
Exposure period: 2 weeks  
Frequency of treatment: daily  
Post. obs. period: no  
Doses: 0.28 or 0.42 ml/kg bw (270 or 400 mg/kg bw)  
Control Group: yes  
Method: GLP: no data  
Year:  
Test substance: other TS: purity 98.4 %  
Remark: 10 animals/sex/group  
Result: no overt signs of toxicity, reduction in conduction velocity of caudal nerve in high dose males, electron microscopic examination showed morphological changes such as retraction of Schwann cell processes surrounding unmyelinated fibres in high dose groups.

20-JAN-1999

(81)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

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Species: rat Sex: male  
Strain: Wistar  
Route of admin.: gavage  
Exposure period: 7 days  
Frequency of treatment: daily  
Post. obs. period: no  
Doses: 140 or 200 mg/kg bw  
Control Group: no data specified  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: purity and group size not mentioned  
Result: marked increments of relative weights of liver and kidneys  
with increase of BUN value and tubular  
degeneration (no further data).

20-JAN-1999

(54)

Species: rat Sex: male  
Strain: Wistar  
Route of admin.: gavage  
Exposure period: one month  
Frequency of treatment: daily  
Post. obs. period: no  
Doses: 130 or 460 mg/kg bw  
Control Group: no data specified  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: purity and group size not mentioned  
Result: marked depression of body weight gain and lethal cases by  
20 and 40 % respectively, tubular damage (no further data).

20-JAN-1999

(54)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

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Species: rat Sex: no data  
Strain: no data  
Route of admin.: dermal  
Exposure period: chronic poisoning  
Frequency of treatment: no data  
Post. obs. period: no data  
Doses: no data  
Control Group: no data specified  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: NOEL: no data  
purity and group size not mentioned  
Result: effects on central nervous system, liver and kidneys (no further data).  
20-JAN-1999 (52)

Species: mouse Sex: male/female  
Strain: CD-1  
Route of admin.: oral feed  
Exposure period: 4 weeks  
Frequency of treatment: daily (feeding study)  
Post. obs. period:  
Doses: 100, 1000, 5000 and 20000 mg/kg diet (15, 150, 750, 3000 mg/kg bw)  
Control Group: yes  
Method:  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: 5/sex/group  
Result: all animals receiving 20000 ppm in diet died or were sacrificed in a moribund condition (failure to eat, hypothermia, dyspnea, lethargy, tremor).  
After 10 days the lowest dietary concentration was changed from 100 ppm to 10000 ppm. No mortality or clinical signs in the 1000, 5000, and 10000 ppm groups. Body weight changes in the 5000 and 10000 ppm groups, increases in liver weight and/or liver weight ratios in male mice at all dose levels and in female mice in the 5000 and 10000 ppm groups, decrease in absolute kidney weight in male mice (10000 ppm).  
20-JAN-1999 (82)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

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Species: mouse Sex: male  
Strain: other: ddy  
Route of admin.: oral feed  
Exposure period: 3 months  
Frequency of treatment: daily (feeding study)  
Post. obs. period: no  
Doses: 500, 2000 and 10000 mg/kg diet (75, 300 and 1500 mg/kg bw)  
Control Group: yes  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: purity and group size not mentioned  
Result: dose-dependent depression of body weight gain, increments of liver, kidney and testis weight, and decrease in uterus weight, no changes in hematological analysis except an increment on BUN value with high level of TBP (no further data).

20-JAN-1999

(54)

Species: mouse Sex: male/female  
Strain: CD-1  
Route of admin.: oral feed  
Exposure period: 3 month  
Frequency of treatment: daily (feeding study)  
Post. obs. period: no  
Doses: 500, 2000 and 8000 mg/kg diet (75, 300 and 1200 mg/kg bw/day)  
Control Group: yes  
Method:  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: 15/sex/group  
Result: All animals survived, in the highest concentration body weight loss and reduced body weight gain with reduced food consumption and reduced fecal volume, elevation of absolute and relative liver weights with hepatocyte hypertrophy, slight to moderate epithelial hyperplasia of the urinary bladder, some slight hematological alterations and some effects on clinical chemistry parameters of liver function. In the middle concentration slight decrease of weight gains, elevated terminal ALT and AST in females and moderately elevated liver weights in both sexes, slight hepatocyte hypertrophy and minimal or slight epithelial hyperplasia of the urinary bladder.  
NOEL: 500 mg/kg bw/day (120 mg/kg bw/day females and 90 mg/kg bw/day males)

20-JAN-1999

(83)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

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Species: rabbit Sex: no data  
Strain: no data  
Route of admin.: inhalation  
Exposure period: 4 months  
Frequency of treatment: 5 days/week, 5 hours/day  
Post. obs. period: 1 month  
Doses: 4.8 or 13.6 mg/m3  
Control Group: no data specified  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: group size and purity not mentioned  
Result: in the high concentration decrease of cholinesterase activity to 33 % after 3 months, effects on physiological and biochemical parameters esp. of the liver. The cholinesterase activity returned to normal in the postexposure period. In the low concentration no effect on cholinesterase activity (no further data).

20-JAN-1999

(52)

Species: rabbit Sex: no data  
Strain: no data  
Route of admin.: gavage  
Exposure period: 14 days  
Frequency of treatment: 7 applications  
Post. obs. period: no data  
Doses: 100, 500 or 1000 mg/kg bw  
Control Group: no data specified  
Method:  
Year: GLP: no  
Test substance: no data  
Remark: purity and size of groups not mentioned  
Result: with 1000 mg/kg transient excretion of protein with urine, no other effects

20-JAN-1999

(67)

## 5. Toxicity

---

Species: other: see remarks Sex: no data  
 Strain: no data  
 Route of admin.: gavage  
 Exposure period: no data  
 Frequency of treatment: daily  
 Post. obs. period: no data  
 Doses: 0.2 to 5 mg/kg/day  
 Control Group: no data specified  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 Remark: NOEL: no data  
 rabbit and rat  
 purity and group size not mentioned  
 Result: liver necrosis, increased liver weight, in one of two  
 studies increased kidney weight and tubulus dystrophia  
 (no further data).  
 20-JAN-1999 (84) (85)

Species: other: see remarks Sex: no data  
 Strain: no data  
 Route of admin.: dermal  
 Exposure period: no data  
 Frequency of treatment: no data  
 Post. obs. period: no data  
 Doses: no data  
 Control Group: no data specified  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 Remark: rat, guinea pig and rabbit  
 Result: purulent-necrotic fissures (no further data).  
 20-JAN-1999 (52)

## 5.5 Genetic Toxicity 'in Vitro'

Type: Ames test  
 System of testing: Salmonella typhimurium TA102 and TA2638 and Escherichia coli  
 WP2/pKM101 and WP2 uvr/pKM101  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method: other: Maron, D.M. and Ames, B.M. (1983)  
 Year: GLP: no data  
 Test substance: no data  
 20-JAN-1999 (86)

## 5. Toxicity

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Type: Ames test  
 System of testing: S. typhimurium TA1535, TA100, TA1537, TA98  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 27-JAN-1999 (87)

Type: Ames test  
 System of testing: S. typhimurium LT-2 (hisC117, hisG46, TA1530, hisD3052, TA1531, TA1532)  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: without  
 Result: negative  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 20-JAN-1999 (88)

Type: Ames test  
 System of testing: S. typhimurium TA1535, TA1538, TA1537, TA98, TA100  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP: no data  
 Test substance: as prescribed by 1.1 - 1.4  
 20-JAN-1999 (89)

Type: Ames test  
 System of testing: S. typhimurium TA1535, TA1538  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: positive  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 27-JAN-1999 (90)

## 5. Toxicity

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Type: Ames test  
 System of testing: no data  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 27-JAN-1999 (91)

Type: Bacterial reverse mutation assay  
 System of testing: E. coli WP2 isogenic strains  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: without  
 Result: negative  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 20-JAN-1999 (88)

Type: Cytogenetic assay  
 System of testing: chinese hamster ovary cells (CHO-K1)  
 Concentration: up to 0.15 ul/ml  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP: yes  
 Test substance: as prescribed by 1.1 - 1.4  
 Remark: chromosome aberration assay  
 20-JAN-1999 (92)

Type: Cytogenetic assay  
 System of testing: mouse embryo, 48 and 144 h post conception  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: without  
 Result: negative  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 Remark: no induction of micronuclei  
 27-JAN-1999 (93)

## 5. Toxicity

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Type: Mammalian cell gene mutation assay  
 System of testing: CHO-K1-BH4 cells  
 Concentration: 0.11, 0.09, 0.08, 0.07, and 0.05 ul/ml without S-9 and 0.15, 0.125, 0.1, 0.08 and 0.06 ul/ml with S-9  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP: yes  
 Test substance: as prescribed by 1.1 - 1.4  
 20-JAN-1999 (94)

## 5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay  
 Species: rat Sex: male/female  
 Strain: no data  
 Route of admin.: gavage  
 Exposure period: single administration  
 Doses: 0, 300, 600, or 1200 mg/kg bw  
 Result:  
 Method:  
 Year: GLP: yes  
 Test substance: as prescribed by 1.1 - 1.4  
 Result: the high dose was the maximum tolerated dose, mortality at the high dose level was 1/15 males and 4/15 females; clinical signs of toxicity at 600 and 1200 mg/kg. No increase of aberrant cells in bone marrow after 12, 24 or 36 hours.  
 20-JAN-1999 (95)

Type: Drosophila SLRL test  
 Species: Drosophila melanogaster Sex:  
 Strain:  
 Route of admin.: oral feed  
 Exposure period:  
 Doses:  
 Result:  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 Remark: 11.1 % lethals; doses not mentioned.  
 Result: negative  
 20-JAN-1999 (88)

5. Toxicity

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## 5.7 Carcinogenicity

Species: rat Sex: male/female  
Strain: Sprague-Dawley  
Route of admin.: oral feed  
Exposure period: 24 months  
Frequency of treatment:  
Post. obs. period:  
Doses: 200, 700 and 3000 ppm  
Result:  
Control Group: yes  
Method: other: US EPA/TSCA  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: Results: There was a dose-related increase in the incidence and severity of hyperplasia and the incidence of papillomas of the urinary bladder epithelium in the mid and high dose groups. Transitional cell carcinomas were noted in the bladders of 6/49 males and 2/50 females in the high dose. A squamous cell carcinoma was noted in the bladder of 1/49 high dose males. The NOEL was 200 ppm TBP in the diet (104 wk mean intake of 8.9 mg/kg/day for males and 11.6 mg/kg/day for females).

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(96)

Species: mouse Sex: male/female  
Strain: CD-1  
Route of admin.: oral feed  
Exposure period: 18 months  
Frequency of treatment:  
Post. obs. period:  
Doses: 150, 1000, 3500 ppm  
Result:  
Control Group: yes  
Method: other: US EPA/TSCA  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: Results: The only histologic change considered to be treatment-related was a statistically significant increase in the incidence of hepatocellular adenoma in high dose male mice. No other tumor type was attributed to TBP administration on the basis of microscopic examinations or statistical analysis. The NOEL for chronic toxicity was 150 ppm (28.9 mg/kg/day for females and 24.1 mg/kg/day for males).

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(97)

## 5. Toxicity

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### 5.8 Toxicity to Reproduction

Type: Two generation study  
Species: rat Sex: male/female  
Strain: Sprague-Dawley  
Route of admin.: oral feed  
Exposure Period:  
Frequency of treatment: daily (feeding study)  
Duration of test: up to two generations  
Doses: 200, 700 and 3000 ppm diet (approx 15, 53 and 225 mg/kg bw/day)  
Control Group: yes  
Method:  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: 30 animals/sex/group  
Result: with 700 and 3000 ppm reductions of body weights, weight gain and food consumption during F0 and F1 prebreed dosing periods, no signs of toxicity, no treatment related mortality; with 200 ppm only transient effects on body weight and food consumption. Urinary bladder epithelial hyperplasia was noted in adults in 700 and 3000 ppm groups in both generations and in F0 males and females and F1 males at 200 ppm. The NOAEL for adult toxicity was <200 ppm based on body weight effects. The NOAEL for reproductive toxicity was >3000 ppm. The NOAEL for post natal toxicity was at or below 200 ppm due to reduced pup weights.

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(98)

### 5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female  
Strain: Sprague-Dawley  
Route of admin.: gavage  
Exposure period: day 6 to 15 of gestation  
Frequency of treatment: daily  
Duration of test: up to day 20 of gestation  
Doses: 80, 435, 790, 1145, and 1500 mg/kg bw  
Control Group: yes  
Method:  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: range-finding study, 5 animals/group  
Result: considerable maternal mortality at dose levels of 790, 1145 and 1500 mg/kg bw. A dose of 80 mg/kg bw was not considered to be maternally toxic, embryotoxic or fetotoxic. At 435 mg/kg bw maternal toxicity but no effect on embryo.

20-JAN-1999

(99)

## 5. Toxicity

Date: 16-APR-2001

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Species: rat Sex: female  
Strain: Wistar  
Route of admin.: gavage  
Exposure period: day 7 to 17 of gestation  
Frequency of treatment: daily  
Duration of test: day 20 of gestation  
Doses: 62.5, 125, 250 or 500 mg/kg/day  
Control Group: yes  
NOAEL Maternalt.: = 62.5 mg/kg bw  
NOAEL Teratogen.: > 250 mg/kg bw  
Method:  
Year: GLP: no data  
Test substance: no data  
Remark: 20 animals/group  
Result: Salivation and depression of body weight gain, adjusted body weight gain and food consumption were observed at the higher doses. There were no significant differences between the groups in the incidence of dead or resorbed fetuses, the number of living fetuses and the body weights of living fetuses of both sexes. The incidence of rudimentary lumbar rib was increased significantly at 500 mg/kg/day. There was one incident of conjoined twins exhibiting three fore-limbs and four hind-limbs at 125 mg/kg/day. This malformation is rare in the background data of teratology, and the incidence of malformed fetuses was not increased significantly. Therefore, TBP was considered not to be teratogenic in this study.

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(100)

Species: rabbit Sex: female  
Strain: other: New Zealand  
Route of admin.: gavage  
Exposure period: day 6 to 18 of gestation  
Frequency of treatment: daily  
Duration of test: up to day 30 of gestation  
Doses: 50, 150 or 400 mg/kg bw  
Control Group: yes  
NOAEL Teratogen.: > 400 mg/kg bw  
Method:  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: 18 animals/group  
Result: at the 400 mg/kg/day dose level maternal toxic effect (mean weight loss and 5% mortality) and no statistically significant increase of resorptions, no fetotoxic or teratogenic effects. At the 50 and 150 mg/kg/day dose level no maternal toxicity, no embryotoxic, fetotoxic or teratogenic effects.

06-APR-1999

(101)

## 5. Toxicity

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Species: rabbit Sex: female  
 Strain: other: New Zealand  
 Route of admin.: gavage  
 Exposure period: day 6 to 18 of gestation  
 Frequency of treatment: daily  
 Duration of test: up to day 30 of gestation  
 Doses: 50, 250, 412, 775, 1137 and 1500 mg/kg bw  
 Control Group: yes  
 Method:  
 Year: GLP: yes  
 Test substance: as prescribed by 1.1 - 1.4  
 Remark: range-finding study, 5 animals/group  
 Result: all animals in the 775, 1137 and 1500 mg groups died during treatment, with 250 and 412 mg/kg maternal mortality 20%, at 50 mg/kg bw no maternal toxicity. No fetotoxicity was evident in the 50, 250 or 412 mg group.

20-JAN-1999 (102)

Species: hen Sex: no data  
 Strain: no data  
 Route of admin.: other  
 Exposure period: single injection in the yolk sac  
 Frequency of treatment:  
 Duration of test:  
 Doses: 5 mg/egg  
 Control Group: yes  
 Method:  
 Year: GLP: no data  
 Test substance: no data  
 Remark: post obs. period: 17 days  
 purity not mentioned  
 Result: weak effects (decrease of survival, weight and length)

27-JAN-1999 (103)

Species: rat Sex: female  
Strain: Sprague-Dawley  
Route of admin.: other: oral  
Exposure period: day 6 to 15 of gestation  
Frequency of treatment: daily  
Duration of test: up to day 20 of gestation  
Doses: 188, 375, or 750 mg/kg bw  
Control Group: yes  
NOAEL Teratogen.: > 750 mg/kg bw  
Method:  
Year: GLP: yes  
Test substance: as prescribed by 1.1 - 1.4  
Remark: 24 animals/group  
Result: in all treatment groups toxicity to dams was produced as evidenced by decrease in absolute body weights and cumulative body weight gains. 29.2 % mortality in the highest dosage group. Treatment related increase in the incidence of delayed skeletal ossification (equivocal biological significance), reduced mean fetal weight in the highest dose group, no teratogenic effects.

20-JAN-1999

(104)

## 5.10 Other Relevant Information

Type: Cytotoxicity  
Remark: Cytotoxicity in vitro: tributyl phosphate inactivated lipid-enveloped viruses, but did not alter the function of serum proteins.

11-SEP-1997

(105)

Type: Cytotoxicity  
Remark: Cytotoxic effects in vitro (HeLa cells)

22-JUL-1997

(106)

Type: Metabolism  
Remark: rat, single i.p. injection of 1 mmol: decrease of glutathione in liver and kidney; small amounts of oxidized butyl moieties were removed as glutathione conjugates and excreted as S-containing metabolites in urine: (3-oxobutyl)- and (3-hydroxybutyl)mercapturic acids (8.9 and 5.2 % of applied dose), other S-butylmercapturic acid derivatives were found only in traces. After i.p. injection of the probable intermediate dibutyl-hydrogenphosphate, only 0.07 and 0.02 % of the applied dose was eliminated as S-containing metabolites in the urine.

22-JUL-1997

(107)

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Type:	Metabolism	
Remark:	(14C-labelled substance was used): - rat, oral: 14 mg/kg: within 1 day, 50 % were excreted in urine, 10 % in exhaled air and 6 % in feces; total elimination after 5 days 82 % - rat, i.p.: 14 mg/kg: within 1 day, 70 % were excreted with urine, 7 % with exhaled air and 4 % in feces; total elimination after 5 days 90 %. - rat, i.p.: 250 mg/kg: 11 phosphorous-containing metabolites in 24-h urine were identified in the neutral and acid fractions with a total recovery of 25 and 12 %. Major metabolites: dibutylhydrogen phosphate(40-64 % of identified dose), butyl dihydrogen phosphate(11-21 % of identified dose), butyl bis (3-hydroxybutyl) phosphate (3-4 % of identified dose) and small amounts of derivatives hydroxylated at the butyl moieties. 1 unidentified neutral metabolite was shown in the gas chromatogram. The butanol-extractable metabolites (25 % of the dose), which were not quantitated, were butyl-3-hydroxybutylphosphate, 3-hydroxybutylphosphate and monobutylphosphate. 47.6 % of dibutyl hydrogenphosphate recovered intact in urine after i.p. infection, therefore the authors concluded that dibutyl hydrogen phosphate produced as an intermediate in the metabolism of tributylphosphate would be mostly excreted. The data after administration of probable metabolic intermediate suggest, that hydroxylation at C-3 is an early metabolic process, which is followed by further metabolic reactions (oxidation to produce carboxylic acids and ketones). The oxo compound (dibutyl 3-oxobutyl phosphate) dibutyl hydrogen phosphate.	
04-NOV-1997		(108)
Type:	Metabolism	
Remark:	cholinesterase inhibition: rat, i.p., 16-266 mg/kg bw (0.062-1 mmole/kg): 21% inhibition of cholinesterase, increased activity of beta-glucuronidase in plasma.	
22-JUL-1997		(109)
Type:	Metabolism	
Remark:	skin of living pigs: hair follicle is not more penetrable than other dermal area; in fact, regions of the skin devoid of follicles were penetrated slightly more rapidly than areas containing follicles.	
22-JUL-1997		(110)
Type:	Metabolism	
Remark:	following single or repeated oral dosing in rats, tributyl phosphate was detected in the gastrointestinal tract, blood and liver (no further data).	
22-JUL-1997		(111)

Type: Metabolism  
Remark: tributyl phosphate is metabolized in rodents to  
butyl-n-cysteine (no further data).  
22-JUL-1997 (112)

Type: Metabolism  
Remark: in vitro: rat liver homogenate: rapid metabolism  
in the presence of NADPH, but only slight breakdown in the  
absence of added NADPH. Dibutyl(3-hydroxybutyl)phosphate  
was obtained as a metabolite in the first stage. The  
extended incubation time yielded two metabolites: butyl  
di(3-hydroxy- butyl)phosphohate and dibutyl hydrogen  
phosphate.  
22-JUL-1997 (113)

Type: Metabolism  
Remark: (14C labelled tributyl phosphate was used):  
rat, single i.v. injection of 5 mg/kg;  
rat, single dermal application of 10 or 350 mg/kg;  
rat, single oral dose of 10 and 350 mg/kg;  
rat, multiple oral dose (8x) of 10 or 350 mg/kg;  
no adverse signs of toxicity in any low dose group, in all  
high dose groups red urine and/or hypersalivation, blood in  
urine in all dose groups. The major proportion of the  
recoverable radioactivity was eliminated within 48 h in  
urine and feces. The major route of elimination is via the  
kidneys (65-85 % of dose after oral and i.v. application).  
The distribution pattern in the tissues was similiar in all  
dose groups. The HPLC analysis showed 9 major and 6 minor  
regions of radioactivity in the urine, mass spectrometric  
analyses revealed monobutylphosphate, dibutylphosphate,  
butyl-2-hydroxybutyl phosphate and  
3-carboxypropyl-dimethylphosphate. The author concluded,  
that the butyl groups of tributylphosphate are oxidized to  
alcoholic, ketonic and acitic functionalities. The oxidized  
chains are also hydrolysed proceeding to the di-, mono- and  
the unsubstituted phosphoric acids.  
04-NOV-1997 (114)

Type: Neurotoxicity  
Remark: hen, oral, two doses of 1500 mg/kg bw  
(LD50) 21 days apart, killed 21 days after the second dose:  
no nerve damage or clinical signs of toxicity (purity  
of test material 98.37%).  
--neurotoxicity: hen, single oral dose of 1500 mg/kg bw:  
no relevant inhibition of brain NTE (neurotoxic esterase)  
or brain actylcholinesterase, increase of plasma cholin-  
esterase (purity of test material 98.37%).  
22-JUL-1997 (57)

## 5. Toxicity

Date: 16-APR-2001

ID: 126-73-8

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Type:	Neurotoxicity	
Remark:	hen, oral: 1840 mg/kg bw on two days: neither behavioral nor histological evidence of neurotoxicity (no further data).	
22-JUL-1997		(51)
Type:	Neurotoxicity	
Remark:	cholinesterase activity in brain and liver homogenates and serum (rat) after incubation with tributyl phosphate (purity > 97 %): no change of enzyme activity	
22-JUL-1997		(77)
Type:	Neurotoxicity	
Remark:	adult hen, oral or dermal 1500 mg/kg bw at day 0 and 21, observation up to day 42: no signs of neuro- toxicity (purity not given).	
22-JUL-1997		(58)
Type:	Neurotoxicity	
Remark:	rat, rabbit: in lethal doses, oral or i.p., decrease of cholinesterase activity in serum, red blood cells, liver and brain of maximum 35 %.	
22-JUL-1997		(52)
Type:	Neurotoxicity	
Remark:	anticholinesterase activity in vitro, human red cell hemolysate or human plasma: slight decrease of cholinesterase activity (purity not mentioned).	
22-JUL-1997		(73)
Type:	Neurotoxicity	
Remark:	range-finding study on motor activity in rats: single oral application of 1000 mg/kg bw, after 0.5 h following dosing, motor activity was tested for 23 hours: one treated female was found dead after 2 days, all treated animals show clinical signs of toxicity, reduced motor activity levels. 4/sex/group purity not known	
22-JUL-1997		(115)
Type:	Neurotoxicity	
Remark:	Neurotoxicity (acute delayed) Hens, single oral dose of 1500 mg/kg with atropine protection. Second TBP dose on day 21. Cholinergic signs including salivation, miosis, and diarrhea. 4 of 20 hens died week 1 and 2, more died on week 2. No ataxia or paralysis. No histopathological lesions.	
23-JUL-1997		(116)
Type:	Neurotoxicity	
Remark:	Result: Not neurotoxic	
	Remarks: Chicken, single 1.84 g/kg oral dose. Repeated dosing at day 21. No signs of neurotoxicity based on locomotor and neuropathology examination.	
23-SEP-1997		(117)

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Type: Neurotoxicity  
Remark: Species: Sprague-Dawley rat  
Route of admin: gavage  
Exposure period: 13 weeks  
Freq. of treatment: daily  
Post. obs. period: no  
Doses: 32, 100 325 mg/kg bw/day  
Control Group: yes  
Test substance: 99.5 %  
Remark: 12 animals/sex/group  
Result: Mortality, salivation and muzzle staining in the 325 mg group and less severe in the 100 mg group, reduced body weight gain, reduced food intake and initial weight loss in the 325 mg group, qualitative functional observational battery assessment did not reveal any significant finding, for quantitative functional observational battery measurements, there were no toxicologically significant differences. Motor activity test results were not significantly different, no abnormal gross pathology findings, neuropathological assessment revealed no effects of treatment.  
30-SEP-1997 (118)

Type: Toxicokinetics  
Remark: Results: Minipig - iv - rapidly eliminated; dermal - poorly absorbed (1-4% excreted); no bioaccumulation in bladder or kidney; metabolism is hydroxylation followed by Phase II (glucuronide, sulfate formation).  
Remarks: iv (5 mg/kg); dermal (10 and 350 mg/kg - 6 hr. exposure)  
04-NOV-1997 (119)

Type: other: Neurotoxic esterase  
Remark: Hens, single dose of 1500 mg/kg. No significant change in brain neurotoxic esterase or acetylcholine esterase activity.  
23-SEP-1997 (120)

Type: other: Neurotoxicity (acute delayed)  
Remark: Hens, dermal exposure 1500 mg/kg day 0-21. No signs of neurotoxicity. No atropine protection.  
23-SEP-1997 (120)

Type: other: Neurotoxicity, acute  
Remark: Results: Not neurotoxic  
Remarks: Rats, doses of 100, 325 and 1000 mg/kg oral. Motor activity and functional observation battery.  
30-SEP-1997 (121)

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Type: other: Subchronic Dietary Mechanistic Study  
Remark: The dose response of TBP effects on the urinary bladder and on urinary parameters was evaluated in male Sprague-Dawley rats fed 0, 200, 700 and 3000 ppm in the diet. Ten rats per group were exposed for 10 weeks. Another group received 3000 ppm TBP plus 12,300 ppm NH<sub>4</sub>Cl. A high dose recovery group (3000 ppm TBP for 10 wks, then 10 wks control diet) was included to evaluate reversibility.

Results: TBP at doses of 700 and 3000 ppm appears to produce urothelial cytotoxicity with marked regenerative hyperplasia. No changes were noted on urinary parameters, other than a slight decrease in osmolality and creatinine at 3000 ppm. Effects were reversible upon withdrawal of treatment during a 10-week recovery period. The toxicity is likely due to the chemical or metabolites, not to urinary changes. A NOEL of 200 ppm was established for all parameters.

28-JUL-1997 (122)

Type:  
Remark: rabbit, i.p.: 100 mg/kg bw single injection: no effect  
200 mg/kg bw single injection: lethal after 11 days  
rabbit, s.c.: 100 or 200 mg/kg bw: no systemic effects, local inflammatory effects.

24-JUL-1997 (67)

Type:  
Remark: no marked difference of LD<sub>50</sub> values observed with oral, s.c. or i.p. administration.

22-JUL-1997 (54)

Type:  
Remark: rat, single oral, i.p. or i.m. application of 0.1 to 0.2 ml: labored breathing, hypersalivation, pallor; paralysis after parenteral application; no symptoms after dermal application (purity not mentioned).

22-JUL-1997 (73)

Type:  
Remark: mice, i.p., 850 - 1000 mg/kg bw: narcosis, muscular paralysis

22-JUL-1997 (123)

Type:  
Remark: Reviews:  
- Environmental Health Criteria 112, World Health Organization (1991)  
- BIBRA Toxicity Profile (1991)  
- Berufsgenossenschaft der chemischen Industrie. Toxikologische Bewertung Ausgabe 02/89, Nr. 170 (1989)

22-JUL-1997

Type:

Remark: rat: eye and nasal irritation after 1 hour exposure to  
atmospheric concentrations of 200 mg/l.

22-JUL-1997 (124)

## 5.11 Experience with Human Exposure

Remark: some decrease in nonspecific esterase  
staining of monocytes in occupational exposed persons.

04-NOV-1997 (125)

Remark: skin penetration in vivo and in vitro:  
maximum steady state penetration rate 0.18 ug/cm<sup>3</sup>/min.

22-JUL-1997 (126)

Remark: workers exposed to 15 mg/m<sup>3</sup> of tributyl phosphate  
have complained of nausea and headache

22-JUL-1997 (127)

Remark: irritant effect on skin and mucous membranes (no  
further data).

11-SEP-1997 (128)

Remark: an abstract of a Soviet paper states that exposure to  
unspecified quantities during the production of scandium  
oxide may have been responsible (together with other  
compounds) for skin rashes in workers (no further  
information)

22-JUL-1997 (129)

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## 7. Risk Assessment

---

### 7.1 End Point Summary

-

### 7.2 Hazard Summary

-

### 7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 107-66-4
CAS No.	107-66-4
EINECS Name	dibutyl hydrogen phosphate
EINECS No.	203-509-8
TSCA Name	Phosphoric acid, dibutyl ester
Molecular Formula	C <sub>8</sub> H <sub>19</sub> O <sub>4</sub> P

Producer Related Part

Company:	
Creation date:	21-JAN-1994

Substance Related Part

Company:	
Creation date:	21-JAN-1994

Memo:	Data for Phosphoric Acid Derivatives Category
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Printing date:	29-JUN-2001
Revision date:	14-FEB-1994
Date of last Update:	14-FEB-2000

Number of Pages:	18
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Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1. General Information

---

### 1.0.1 OECD and Company Information

-

### 1.0.2 Location of Production Site

-

### 1.0.3 Identity of Recipients

-

## 1.1 General Substance Information

Substance type: inorganic

Physical status: liquid

### 1.1.0 Details on Template

-

### 1.1.1 Spectra

-

## 1.2 Synonyms

DI-N-BUTYL PHOSPHATE

DIBUTYL HYDROGEN PHOSPHATE

DIBUTYL PHOSPHATE

PHOSPHORIC ACID, DIBUTYL ESTER

## 1.3 Impurities

-

## 1.4 Additives

-

## 1.5 Quantity

Quantity

1. General Information

---

## 1.6.1 Labelling

## 1.6.2 Classification

## 1.7 Use Pattern

Type: type  
Category: Non dispersive use

Type: industrial  
Category: Chemical industry: used in synthesis

Type: use  
Category: Intermediates

## 1.7.1 Technology Production/Use

-

## 1.8 Occupational Exposure Limit Values

-

## 1.9 Source of Exposure

-

## 1.10.1 Recommendations/Precautionary Measures

-

## 1.10.2 Emergency Measures

-

## 1.11 Packaging

-

1. General Information

---

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

1.14.2 Major Accident Hazards

1.14.3 Air Pollution

1.15 Additional Remarks

-

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

---

## 2.1 Melting Point

Value: ca. -13 degree C (1)

## 2.2 Boiling Point

Value: > 200 degree C at 20 hPa  
Decomposition: yes (1)

## 2.3 Density

Type: density  
Value: 1.05 g/cm3 at 20 degree C (1)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

Value: < .1 hPa at 20 degree C (1)

## 2.5 Partition Coefficient

log Pow: .6 - 1.4  
Method: other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989.  
Daylight, Chemical Information Systems, Claremont, CA 91711,  
USA  
Year: (2)

log Pow: 2.2889  
Method: other (calculated): KOWWIN Program, version 1.65  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure (16)

## 2.6.1 Water Solubility

Value: 18 g/l at 20 degree C (1)

## 2.6.2 Surface Tension

-

2. Physico-chemical Data

---

## 2.7 Flash Point

Value: 188 degree C  
Type: other  
Method: other: DIN 51376  
Year:

(1)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Additional Remarks

Remark: pK value: 1.17

(3)

## 3. Environmental Fate and Pathways

## 3.1.1 Photodegradation

Type: air

## INDIRECT PHOTOLYSIS

Sensitizer: OH

Conc. of sens.: 1560000 molecule/cm3

Rate constant: 52.6999 E-12 cm3/(molecule \* sec)

Degradation: 50 % after 2.436 hour(s)

Method: other (calculated): AOP Program (v1.89)

Year: 1999

GLP: no

Test substance: other TS: molecular structure

(16)

## 3.1.2 Stability in Water

-

## 3.1.3 Stability in Soil

-

## 3.2 Monitoring Data (Environment)

-

## 3.3.1 Transport between Environmental Compartments

Type: fugacity model level III

Media: other: air - water - soil - sediment

Air (Level I):

Water (Level I):

Soil (Level I):

Biota (L.II/III):

Soil (L.II/III):

Method: other: Level III Fugacity Model

Year:

Result:	Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
	Air	0.183	4.87	1000	1.58e-012
	Water	34.4	208	1000	2.65e-014
	Soil	65.3	208	1000	2.52e-013
	Sediment	0.112	832	0	1.48e-014

Persistence Time: 253 hr

Reaction Time: 279 hr

Advection Time: 2.76e+003 hr

Percent Reacted: 90.8

Percent Advected: 9.2

Remark: Default input values of 1000 kg/hr were used for model.

(16)

## 3.3.2 Distribution

-

3. Environmental Fate and Pathways

---

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

Type:

Inoculum: predominantly domestic sewage

Concentration: 4.4 mg/l

Degradation: 12 % after 28 day

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"

Year:

GLP:

Test substance:

Remark: related to BOD

(4)

Type:

Inoculum:

7 day 9 %

14 day 97 %

21 day &gt; 98 %

28 day &gt; 98 %

Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"

Year:

GLP:

Test substance:

(4)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

-

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

Type:  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC0: >= 100  
Method: other: Akute Toxizitaet fuer Fische (C.1.), Richtlinie  
67/548/EWG (Entwurf 1992)  
Year: GLP:  
Test substance:

(4)

Type:  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC0: > 10000  
Method: other: Letale Wirkung beim Zebrabaerbling,  
UBA-Verfahrensvorschlag, Mai 1984, Letale Wirkung beim  
Zebrabaerbling Brachydanio rerio LC0, LC50, LC100, 48-96h  
Year: GLP:  
Test substance:  
Remark: direct weight

(4)

Type: other: calculation  
Species: other: fish  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
LC50: 83.187  
Method: other: ECOSAR Program (v0.99e)  
Year: 1999 GLP: no  
Test substance: other TS: molecular structure

(16)

## 4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculation  
Species: Daphnia sp. (Crustacea)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring: no  
LC50 : 90.941  
Method: other: ECOSAR Program (v0.99e)  
Year: 1999 GLP: no  
Test substance: other TS: molecular structure

(16)

#### 4. Ecotoxicity

---

##### 4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae  
Endpoint:  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring: no  
EC50: 57.811  
Method: other: ECOSAR Program (v0.99e)  
Year: 1999 GLP: no  
Test substance: other TS: molecular structure

(16)

##### 4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic  
Species: activated sludge  
Exposure period: 3 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: > 10000  
Method: ISO 8192 "Test for inhibition of oxygen consumption by  
activated sludge"  
Year: GLP:  
Test substance:  
Remark: direct weight

(4)

##### 4.5 Chronic Toxicity to Aquatic Organisms

###### 4.5.1 Chronic Toxicity to Fish

-

###### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

##### TERRESTRIAL ORGANISMS

###### 4.6.1 Toxicity to Soil Dwelling Organisms

-

###### 4.6.2 Toxicity to Terrestrial Plants

-

###### 4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

-

##### 4.7 Biological Effects Monitoring

-

##### 4.8 Biotransformation and Kinetics

-

##### 4.9 Additional Remarks

-

5. Toxicity

---

## 5.1 Acute Toxicity

## 5.1.1 Acute Oral Toxicity

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: = 3200 mg/kg bw  
Method:  
Year:  
Test substance:

GLP:

(5)

Type: LD50  
Species: rat  
Strain:  
Sex: male/female  
Number of  
Animals: 5  
Vehicle: no data  
Value: > 2000 mg/kg bw  
Method: OECD Guide-line 401 "Acute Oral Toxicity"  
Year: GLP: yes  
Test substance: other TS  
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and  
other 19.1%

15-APR-1999

(6)

## 5.1.2 Acute Inhalation Toxicity

-

## 5.1.3 Acute Dermal Toxicity

-

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: highly irritating

EC classificat.:

Method: other: see remarks

Year:

GLP:

Test substance:

Remark: method: ear, exposure time: 8 h, dose: 500 ul/animal, semi-occlusive, postexposure observation period: 7 d

(7)

## 5.2.2 Eye Irritation

Species: rabbit

Concentration:

Dose:

Exposure Time:

Comment:

Number of

Animals:

Result: highly irritating

EC classificat.:

Method: other: see remarks

Year:

GLP:

Test substance:

Remark: method: dose: 100 ul/animal, postexposure observation period: 7 d

test substance causes corrosion of the cornea

(7)

## 5. Toxicity

Date: 29-JUN-2001

ID: 107-66-4

### 5.3 Sensitization

Type: Guinea pig maximization test  
 Species: guinea pig  
 Concentration: Induction 1 % intracutaneous  
 Induction 10 % occlusive epicutaneous  
 Challenge 2 % occlusive epicutaneous  
 Number of  
 Animals: 10  
 Vehicle: water  
 Result: not sensitizing  
 Classification:  
 Method: OECD Guide-line 406 "Skin Sensitization"  
 Year: 1999 GLP: yes  
 Test substance: other TS: purity 99,4%  
 Remark: 5 animals in control group  
 14-FEB-2000

(8)

### 5.4 Repeated Dose Toxicity

Species: rat Sex: male/female  
 Strain: Sprague-Dawley  
 Route of admin.: gavage  
 Exposure period: 44 days (male) and from 14 days before mating to day 3 of lactation (females)  
 Frequency of treatment: daily  
 Post. obs. period: no  
 Doses: 0, 30, 100, 300 and 1000 mg/kg  
 Control Group: yes  
 NOAEL: 30 mg/kg bw  
 Method: other  
 Year: 1995 GLP: yes  
 Test substance: other TS  
 Method: OECD Guideline 422  
 Remark: Number of animals: 10/sex/group; Vehicle: sesame oil  
 Result: transient red urine and a decrease in food consumption with >= 100 mg/kg (males). 3 males and 2 females died in the 1000 mg/kg-group. No effects on urinary, hematological and blood chemical findings in the males (females not given). Histopathology showed epithelial hyperplasia accompanied by degeneration and ulceration of the urinary bladder mucosa in males and females with >= 100 mg/kg. Epithelial hyperplasia and hyperkeratosis of the forestomach (some with erosion and ulceration in the gastric mucosa) were noted in both sexes >= 300 mg/kg. Increase of absolute and relative liver weight and hepatocellular swelling in females with 1000 mg/kg. NOEL 30 mg/kg bw. For reproductive effects see 5.8.  
 Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%

15-APR-1999

(6)

## 5. Toxicity

Date: 29-JUN-2001

ID: 107-66-4

Species: hen Sex: no data  
 Strain: no data  
 Route of admin.: dermal  
 Exposure period: 90 d  
 Frequency of treatment:  
 Post. obs. period: no data  
 Doses: 100 mg/kg bw/d  
 Control Group: no data specified  
 Method:  
 Year: GLP:  
 Test substance:  
 Remark: purity not known  
 Result: delayed neurotoxic effects (no details, no further data)

(9)

### 5.5 Genetic Toxicity 'in Vitro'

Type: Ames test  
 System of testing: S. typhimurium TA100, TA1535, TA98, TA1537, E.coli WP2uvrA  
 Concentration: 0 - 156.2 µg/plate  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method: other  
 Year: 1995 GLP: yes  
 Test substance: other TS  
 Method: Guideline for Screening Mutagenicity Testing of Chemicals (Japan)  
 Remark: plate incorporation assay, vehicle acetone, toxicity was observed with 156.2 µg/plate  
 Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%

15-APR-1999

(6)

Type: Ames test  
 System of testing: S. typhimurium TA 1535, TA 1537, TA 98, TA 100  
 Concentration:  
 Cytotoxic Conc.:  
 Metabolic activation: with and without  
 Result: negative  
 Method:  
 Year: GLP:  
 Test substance:

(10)

## 5. Toxicity

---

Type: Cytogenetic assay  
System of testing: Chinese hamster CHL/IU cells  
Concentration: 0 - 0.54 mg/ml  
Cytotoxic Conc.:  
Metabolic activation: with and without  
Result: negative  
Method: other  
Year: 1995 GLP: yes  
Test substance: other TS  
Method: Guideline for Screening Mutagenicity Testing of Chemicals (Japan)  
Remark: no clastogenicity, no polyploidy, tested up to 50% growth inhibition  
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%  
16-APR-1999 (6)

## 5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay  
Species: mouse Sex: male/female  
Strain: NMRI  
Route of admin.: gavage  
Exposure period: twice at an interval of 24 hours  
Doses: 0, 100, 300, 1000 mg/kg bw  
Result: negative  
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"  
Year: 1999 GLP: yes  
Test substance: other TS: purity 99,4%  
Remark: Number of animals: 5/sex/group; vehicle: deionized water  
Result: 1000mg/kg bw caused death in 2 females with macroscopic findings of orange spume in gastro-intestinal tract; these 2 females were replaced and survived after treatment; motor activity was decreased in group 1000mg/kg bw; ratio of polychromatic erythrocytes to total erythrocytes was not changed to a significant extent  
14-FEB-2000 (11)

## 5.7 Carcinogenicity

-

## 5.8 Toxicity to Reproduction

Type: other  
Species: rat Sex: male/female  
Strain: Sprague-Dawley  
Route of admin.: gavage  
Exposure Period: 44 days (male) and from 14 days before mating to day 3 of lactation (females)  
Frequency of treatment: daily  
Duration of test:  
Doses: 0, 30, 100, 300 and 1000 mg/kg  
Control Group: yes  
Method: other  
Year: 1995 GLP: yes  
Test substance: other TS  
Method: OECD Guideline 422  
Remark: Number of animals: 10/sex/group; Vehicle: sesame oil  
Result: transient red urine and a decrease in food consumption with  $\geq 100$  mg/kg (males). 3 males and 2 females died in the 1000 mg/kg-group. Epithelial hyperplasia accompanied by degeneration and ulceration of the urinary bladder mucosa in males and females with  $\geq 100$  mg/kg. Epithelial hyperplasia and hyperkeratosis of the forestomach (some with erosion and ulceration in the gastric mucosa) were noted in both sexes  $\geq 300$  mg/kg. Increase of absolute and relative liver weight and hepatocellular swelling in females with 1000 mg/kg. No significant effects on reproductive parameters including copulation index, fertility index, number of corpora lutea and implantation sites, gestation index and gestation length. The number of live pups and the viability index decreased with 1000 mg/kg, attributable to the high incidence of fatalities of pups in some litters at or after birth.  
Test substance: purity 62.6%, other contents: monoester 18.3%, triester and other 19.1%

15-APR-1999

(6)

## 5.9 Developmental Toxicity/Teratogenicity

-

## 5.10 Other Relevant Information

Type: Metabolism  
Remark: rat, single i.p. infection of 250 mg/kg:  
only 0.072 and 0.023 % of the applied dose was found in the urine as S-containing metabolites.

(12)

Type:

Remark:

Metabolism:

after i.p.-administration of the pesticide aminophon (O,O-di- n-butyl-1-n-butyl-amino-cyclohexyl-phosphonate) to rats, dibutylphosphate was detectable in the urine among other metabolites; orally administered aminophon also yielded dibutylphosphate, but to a lesser amount, in the urine.

(13)

Type:

Remark:

Metabolism:

after a single i.p.-administration of tributyl phosphate at a dose of 250 mg/kg bw to male rats, dibutyl phosphate was identifiable in the 24-h urine among other phosphorus-containing metabolites. When rats were dosed with dibutyl phosphate, 47.6 % was recovered intact in the urine.

(14)

Type:

Remark:

Metabolism:

in vitro-study: prolonged incubation of tributylphosphate with rat liver 9000 g supernatant: dibutylphosphate was detectable among other metabolites (amount of dibutylphosphate: 3 % of the applied substrate=tributylphosphate).

(15)

#### 5.11 Experience with Human Exposure

Remark:

workers exposed to unspecified concentrations of vapor complained of respiratory irritation and headache (no further data).

(5)

6. References

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## 7. Risk Assessment

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### 7.1 End Point Summary

-

### 7.2 Hazard Summary

-

### 7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical ID: 298-07-7  
CAS No. 298-07-7  
EINECS Name bis(2-ethylhexyl) hydrogen phosphate  
EINECS No. 206-056-4  
TSCA Name Phosphoric acid, bis(2-ethylhexyl) ester  
Molecular Formula C16H35O4P

Producer Related Part

Company:  
Creation date: 16-OCT-2001

Substance Related Part

Company:  
Creation date: 16-OCT-2001

Memo: Data for Phosphoric Acid Derivatives Category

Printing date: 16-OCT-2001  
Revision date:  
Date of last Update: 16-OCT-2001

Number of Pages: 19

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7  
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4  
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

---

## 1.0.1 OECD and Company Information

-

## 1.0.2 Location of Production Site

-

## 1.0.3 Identity of Recipients

-

## 1.1 General Substance Information

Substance type: inorganic  
Physical status: liquid  
Source: Bayer AG Leverkusen  
24-AUG-1992

## 1.1.0 Details on Template

-

## 1.1.1 Spectra

-

## 1.2 Synonyms

BIS(2-ETHYLHEXYL) HYDROGEN PHOSPHATE  
Source: Bayer AG Leverkusen  
03-AUG-1992

BIS(2-ETHYLHEXYL) PHOSPHATE  
Source: Bayer AG Leverkusen  
03-AUG-1992

BIS(2-ETHYLHEXYL) PHOSPHORIC ACID  
Source: Bayer AG Leverkusen  
03-AUG-1992

DI(2-ETHYLHEXYL) PHOSPHORIC ACID  
Source: Bayer AG Leverkusen  
03-AUG-1992

DI-2-ETHYLHEXYL HYDROGEN PHOSPHATE  
Source: Bayer AG Leverkusen  
03-AUG-1992

DIOCTYLPHOSPHAT  
Source: Bayer AG Leverkusen  
03-AUG-1992

1. General Information

---

PHOSPHORIC ACID BIS(ETHYLHEXYL) ESTER  
Source: Bayer AG Leverkusen  
03-AUG-1992

PHOSPHORIC ACID, BIS(2-ETHYLHEXYL) ESTER  
Source: Bayer AG Leverkusen  
03-AUG-1992

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

-

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

-

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

-

1.9 Source of Exposure

1.10.1 Recommendations/Precautionary Measures

-

1. General Information

---

1.10.2 Emergency Measures

-

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

-

1.14.2 Major Accident Hazards

-

1.14.3 Air Pollution

-

1.15 Additional Remarks

-

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

---

## 2.1 Melting Point

Value: ca. -50 degree C  
Source: Bayer AG Leverkusen  
16-OCT-2001 (1)

Value: 86.3 degree C  
Method: other: MPBPWIN (v1.31)  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Melting Point: 75.00 deg C (Adapted Joback Method)  
Melting Point: 120.14 deg C (Gold and Ogle Method)  
Mean Melt Pt : 97.57 deg C (Joback; Gold,Ogle Methods)  
Selected MP: 86.28 deg C (Weighted Value)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
16-OCT-2001 (2)

## 2.2 Boiling Point

Value: 240 degree C at 1013 hPa  
Decomposition: yes  
Source: Bayer AG Leverkusen  
16-OCT-2001 (3)

Value: 400.4 degree C at 1013 hPa  
Method: other: MPBPWIN Program (version 1.31) Adapted Stein and Brown  
Method  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Reliability: (2) valid with restrictions  
Accepted calculation method  
16-OCT-2001 (2)

## 2.3 Density

Type: density  
Value: .96 g/cm3 at 20 degree C  
Source: Bayer AG Leverkusen  
26-AUG-1992 (1)

## 2.3.1 Granulometry

-

2. Physico-chemical Data

---

## 2.4 Vapour Pressure

Value: < .1 hPa at 20 degree C  
Source: Bayer AG Leverkusen  
26-AUG-1992 (1)

Value: .00000006199 hPa at 25 degree C  
Method: other (calculated): MPBPWIN (v1.31)  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Vapor Pressure Estimations (25 deg C):  
(Using BP: 400.41 deg C (estimated))  
(Using MP: 86.28 deg C (estimated))  
VP: 7.09E-009 mm Hg (Antoine Method)  
VP: 4.65E-008 mm Hg (Modified Grain Method)  
VP: 4.13E-006 mm Hg (Mackay Method)  
Selected VP: 4.65E-008 mm Hg (Modified Grain Method)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
16-OCT-2001 (2)

## 2.5 Partition Coefficient

log Pow: 6.071 at 25 degree C  
Method: other (calculated)  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Reliability: (2) valid with restrictions  
Accepted calculation method  
16-OCT-2001 (2)

log Pow: 4.6 - 5.4  
Method: other (calculated): Leo, A.: CLOGP-3.54 MedChem Software 1989.  
Daylight, Chemical Information Systems, Claremont, CA 91711,  
USA  
Year:  
Source: Bayer AG Leverkusen  
16-OCT-2001 (4)

2. Physico-chemical Data

---

## 2.6.1 Water Solubility

Value: .05926 mg/l at 25 degree C  
Method: other: WSKOW (v1.36)  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Log Kow (estimated) : 6.07  
Log Kow (experimental): not available from database  
Log Kow used by Water solubility estimates: 6.07

Equation Used to Make Water Sol estimate:

$$\text{Log S (mol/L)} = 0.796 - 0.854 \log \text{Kow} - 0.00728 \text{ MW}$$

Log Water Solubility (in moles/L) : -6.736

Water Solubility at 25 deg C (mg/L): 0.05926

Reliability: (2) valid with restrictions

Accepted calculation method

16-OCT-2001

(2)

Value: < 1 g/l  
Source: Bayer AG Leverkusen

16-OCT-2001

(1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

Value: ca. 198 degree C  
Type: closed cup  
Method: other: DIN 51758  
Year:  
Source: Bayer AG Leverkusen  
26-AUG-1992

(1)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

2.12 Additional Remarks

-

## 3. Environmental Fate and Pathways

## 3.1.1 Photodegradation

Type: air  
 INDIRECT PHOTOLYSIS  
 Sensitizer: OH  
 Conc. of sens.: 1560000 molecule/cm3  
 Rate constant: .0000000000653784 cm3/(molecule \* sec)  
 Degradation: 50 % after 2 hour(s)  
 Method: other (calculated): AOP Program (v1.89)  
 Year: 1999 GLP: no  
 Test substance: other TS: molecular structure  
 Reliability: (2) valid with restrictions  
 Accepted calculation method

16-OCT-2001

(2)

## 3.1.2 Stability in Water

-

## 3.1.3 Stability in Soil

-

## 3.2 Monitoring Data (Environment)

-

## 3.3.1 Transport between Environmental Compartments

Type: fugacity model level III  
 Media: other: air - water - soil - sediment  
 Air (Level I):  
 Water (Level I):  
 Soil (Level I):  
 Biota (L.II/III):  
 Soil (L.II/III):  
 Method: other: Level III Fugacity Model  
 Year: 1999  
 Result:

Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.278	3.93	1000	5.89e-013
Water	12.9	360	1000	7.45e-014
Soil	36.7	360	1000	3.64e-016
Sediment	50.1	1.44e+003	0	2.24e-014

Persistence Time: 540 hr

Reaction Time: 593 hr

Advection Time: 6e+003 hr

Percent Reacted: 91

Percent Advected: 8.99

Remark: Default input values of 1000 kg/hr were used for model.

Reliability: (2) valid with restrictions

Accepted calculation method

16-OCT-2001

(2)

3. Environmental Fate and Pathways

---

## 3.3.2 Distribution

-

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

## Type:

Inoculum: predominantly domestic sewage

Degradation: 0 % after 5 day

Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"

Year:

GLP:

Test substance:

Remark: related to BOD

Source: Bayer AG Leverkusen

Reliability: (1) valid without restriction  
Guideline study

16-OCT-2001

(3)

## Type:

Inoculum: predominantly domestic sewage

Concentration: 100 mg/l

Degradation: 75 % after 28 day

Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"

Year:

GLP:

Test substance:

Remark: related to O2-demand

Source: Bayer AG Leverkusen

Reliability: (2) valid with restrictions  
Meets National standards

16-OCT-2001

(3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

-

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

Type: static  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: > 56  
Method: ISO 7346/1-3  
Year: 1975 GLP: no data  
Test substance: other TS: di-(2-ethyl hexyl)-phosphoric acid; purity not stated  
Method: Exceptions to the ISO protocol: water temperature was kept at 25 degree C and the exposure period was extended to 144 hours (without renewal of toxicant).  
Result: Exposure 24 hr 48 hr 144 hr  
LC50 (mg/l) >56.0 >56.0 >56.0  
Reliability: (1) valid without restriction  
Meets National standards  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (5)

Type: static  
Species: Salmo gairdneri (Fish, estuary, fresh water)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
LC50: 30  
Method: GLP:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
Test condition: at 15 degree C  
26-AUG-1992 (6)

Type: static  
Species: Leuciscus idus (Fish, fresh water)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
LC0: 20  
LC100: 40  
Method: other: Bestimmung der akuten Wirkung von Stoffen auf Fische. Arbeitskreis "Fischtest" im Hauptausschuss "Detergentien" (15.10.73)  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
11-FEB-1993 (3)

#### 4. Ecotoxicity

Date: 16-OCT-2001  
ID: 298-07-7

Type: semistatic  
Species: Brachydanio rerio (Fish, fresh water)  
Exposure period: 10 day  
Unit: mg/l Analytical monitoring:  
LT50 : 21  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
26-AUG-1992 (5)

Type: semistatic  
Species: other: Oncorhynchus mykiss, eye pointed embryo  
Exposure period: 48 day  
Unit: mg/l Analytical monitoring:  
LT50 : 20.6  
Method:  
Year: GLP:  
Test substance:  
Remark: Diluting agent: Acetone removed before the start of the test  
Source: Bayer AG Leverkusen  
05-AUG-1993 (5)

#### 4.2 Acute Toxicity to Aquatic Invertebrates

Type: static  
Species: Daphnia magna (Crustacea)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: > 42.0  
Method: other  
Year: GLP: no data  
Test substance: other TS: di-(2-ethyl hexyl)-phosphoric acid; purity not stated  
Result: Exposure 24 hr 48 hr 72 hr 96 hr  
LC50 (mg/l) >42.0 >42.0 46.8 27.2  
95% conf. limit (19.8-110) (9.6-77.2)  
Upper confidence limit was highest concentration tested.  
Test condition: Medium: Standard Reference water (ISO 1977)  
Temperature: 20-23 degree C  
Illumination: diffuse light 12 hr per day  
No food was added during the test  
Reliability: (2) valid with restrictions  
Meets generally accepted scientific standards, well documented and acceptable for assessment.  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (5)

#### 4. Ecotoxicity

Date: 16-OCT-2001  
ID: 298-07-7

---

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 48 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 60.7  
Method: other: static  
Year: GLP:  
Test substance:  
Remark: diluting agent: Acetone  
Source: Bayer AG Leverkusen  
05-AUG-1993 (7)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 72 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 36.5  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992 (6)

Type:  
Species: Daphnia magna (Crustacea)  
Exposure period: 96 hour(s)  
Unit: mg/l Analytical monitoring:  
EC50: 16.5  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992 (6)

#### 4.3 Toxicity to Aquatic Plants e.g. Algae -

#### 4.4 Toxicity to Microorganisms e.g. Bacteria

Type:  
Species: Pseudomonas fluorescens (Bacteria)  
Exposure period: 24 hour(s)  
Unit: mg/l Analytical monitoring:  
EC0: 2500  
Method: other: Bestimmung der biologischen Schadwirkung toxischer  
Abwaesser gegen Bakterien. DEV, L 8 (1968) modifiziert  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
26-AUG-1992 (3)

4. Ecotoxicity

---

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

-

4.6.2 Toxicity to Terrestrial Plants

-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

-

4.7 Biological Effects Monitoring

-

4.8 Biotransformation and Kinetics

-

4.9 Additional Remarks

-

5. Toxicity

---

## 5.1 Acute Toxicity

## 5.1.1 Acute Oral Toxicity

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Value: 4940 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992

(8)

## 5.1.2 Acute Inhalation Toxicity

-

## 5.1.3 Acute Dermal Toxicity

-

## 5.1.4 Acute Toxicity, other Routes

Type: LD50  
Species: rat  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.p.  
Value: 50 - 100 mg/kg bw  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992

(9)

5. Toxicity

---

Type: LD50  
Species: rabbit  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.p.  
Value: 1250 mg/kg bw  
Method:  
Year:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992

GLP:

(8)

Type: LDLo  
Species: mouse  
Strain:  
Sex:  
Number of  
Animals:  
Vehicle:  
Route of admin.: i.p.  
Value: 63 mg/kg bw  
Method:  
Year:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992

GLP:

(10)

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

Species: rabbit  
Concentration:  
  
Exposure:  
Exposure Time:  
Number of  
Animals:  
PDII:  
Result: corrosive  
EC classificat.:  
Method: other: see remarks  
Year:  
Test substance:  
Remark: 2 animals, 500 ul/animal, 1-8 h exposure time,  
Post exposure time 7 d  
Source: Bayer AG Leverkusen  
26-AUG-1992

GLP:

(11)

5. Toxicity

---

Species: other: no data  
Concentration:

Exposure:  
Exposure Time:  
Number of  
Animals:

PDII:

Result: corrosive

EC classificat.:

Method: other: no data

Year:

GLP:

Test substance:

Source: Bayer AG Leverkusen  
03-AUG-1992

(12)

## 5.2.2 Eye Irritation

Species: rabbit

Concentration:

Dose:

Exposure Time:

Comment:

Number of

Animals:

Result: corrosive

EC classificat.:

Method: other: see remarks

Year:

GLP:

Test substance:

Remark: 2 animals, 100ul/animal, post exposure time 7 d;

Source: Bayer AG Leverkusen

26-AUG-1992

(11)

## 5.3 Sensitization

-

## 5.4 Repeated Dose Toxicity

-

5. Toxicity

---

## 5.5 Genetic Toxicity 'in Vitro'

Type: Ames test  
System of testing: S. typhimurium TA 98, TA100, TA 1535, TA1537  
Concentration:  
Cytotoxic Conc.:  
Metabolic activation: with and without  
Result: negative  
Method:  
Year: GLP:  
Test substance:  
Source: Bayer AG Leverkusen  
03-AUG-1992

(13)

## 5.6 Genetic Toxicity 'in Vivo'

-

## 5.7 Carcinogenicity

-

## 5.8 Toxicity to Reproduction

-

## 5.9 Developmental Toxicity/Teratogenicity

-

## 5.10 Other Relevant Information

Type:  
Remark: Induction of liver enzyme activity (peroxisome proliferation, induction of epoxid hydrolase)  
Source: Bayer AG Leverkusen  
03-AUG-1992

(14) (15)

## 5.11 Experience with Human Exposure

-

6. References

---

- (1) Safety Data Sheet Bayer AG 15.05.1987
- (2) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center. 6225 Running Ridge Road, North Syracuse, NY 13212-2510
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## 7. Risk Assessment

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### 7.1 End Point Summary

-

### 7.2 Hazard Summary

-

### 7.3 Risk Assessment

-

I U C L I D

D a t a S e t

New Chemical ID: 12645-31-7  
CAS No. 12645-31-7  
TSCA Name 2-ethylhexyl phosphate  
Molecular Weight 210.21  
Molecular Formula C8 H19 O4 P1

Producer Related Part  
Company:  
Creation date: 27-JUN-2001

Substance Related Part  
Company:  
Creation date: 27-JUN-2001

Memo: Phosphoric Acid Derivatives Panel

Printing date: 28-NOV-2001  
Revision date:  
Date of last Update: 28-NOV-2001

Number of Pages: 17

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7  
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4  
Flags (profile): Flags: without flag, confidential, non confidential, WGK  
(DE), TA-Luft (DE), Material Safety Dataset, Risk  
Assessment, Directive 67/548/EEC, SIDS

1. General Information

---

## 1.0.1 OECD and Company Information

Type: lead organisation  
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Phosphoric Acid Derivatives Panel  
Street: Wilson Boulevard  
Town: 22209 Arlington, VA  
Country: United States  
Phone: 703-741-5600  
Telefax: 703-741-6091

16-OCT-2001

Type: cooperating company  
Name: Bayer Corporation  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: Baker Petrolite Corporation  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: Crompton Corporation  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: ICI Americas (Uniqema)  
Country: United States

16-OCT-2001

Type: cooperating company  
Name: Noveon, Inc. (formerly BF Goodrich)  
Country: United States

16-OCT-2001

## 1.0.2 Location of Production Site

-

## 1.0.3 Identity of Recipients

-

## 1.1 General Substance Information

-

1. General Information

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1.1.0 Details on Template

-

1.1.1 Spectra

-

1.2 Synonyms

-

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

-

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

-

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

-

1.9 Source of Exposure

-

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1. General Information

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1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

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1.13 Statements Concerning Waste

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1.14.1 Water Pollution

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1.14.2 Major Accident Hazards

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1.14.3 Air Pollution

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1.15 Additional Remarks

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1.16 Last Literature Search

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1.17 Reviews

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1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

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## 2.1 Melting Point

Value: 81.3 degree C  
Method: other: MPBPWIN Program, version 1.31  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Melting Point: 69.26 deg C (Adapted Joback Method)  
Melting Point: 93.33 deg C (Gold and Ogle Method)  
Mean Melt Pt : 81.30 deg C (Joback; Gold,Ogle Methods)  
Selected MP: 81.30 deg C (Mean Value)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
27-JUN-2001 (1)

## 2.2 Boiling Point

Value: 354.5 degree C at 1013 hPa  
Method: other: MPBPWIN Program, version 1.31  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Result: Boiling Point: 354.51 deg C (Adapted Stein and Brown Method)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
22-OCT-2001 (1)

Value: > 93 degree C  
27-JUN-2001 (2)

Value:  
Decomposition: yes  
27-JUN-2001 (3)

## 2.3 Density

Type:  
Value: 1.05 g/cm3 at 20 degree C  
Testsubstance: other TS: 2-ethylhexyl phosphate; purity = 98%  
27-JUN-2001 (3)

## 2.3.1 Granulometry

-

## 2. Physico-chemical Data

## 2.4 Vapour Pressure

Value: .000000712 hPa at 25 degree C  
 Method: other (calculated): MPBPWIN Program, version 1.31  
 Year: 1999  
 GLP: no  
 Testsubstance: other TS: molecular structure  
 Result: Vapor Pressure Estimations (25 deg C):  
         (Using BP: 354.51 deg C (estimated))  
         (Using MP: 81.30 deg C (estimated))  
             VP: 1.9E-007 mm Hg (Antoine Method)  
             VP: 5.34E-007 mm Hg (Modified Grain Method)  
             VP: 5.7E-005 mm Hg (Mackay Method)  
             Selected VP: 5.34E-007 mm Hg (Modified Grain Method)  
 Reliability: (2) valid with restrictions  
             Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (1)

Value:  
 Remark: nonvolatile  
 27-JUN-2001 (3)

## 2.5 Partition Coefficient

log Pow: 2.65  
 Method: other (calculated): KOWWIN Program, version 1.65  
 Year: 1999  
 GLP: no  
 Testsubstance: other TS: molecular structure  
 Reliability: (2) valid with restrictions  
             Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 27-JUN-2001 (1)

## 2.6.1 Water Solubility

Qualitative: other: dispersible  
 Remark: We attempted to make a water solution of CASRN 12645-31-7  
         (Phosphoric acid, 2-ethylhexyl ester).  
         Even at 400 ppm, the product was obviously water insoluble. A  
         cosolvent, isopropyl alcohol, which is allowed at a <1% level  
         was tried but did not help. Even at 40 ppm, the product does  
         not appear to be soluble. The bottom line is that the product  
         is simply not water soluble enough to make a solution which  
         could be adequately quantitated for determination of  
         hydrolysis.  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (4) (2)

## 2. Physico-chemical Data

Date: 22-OCT-2001

ID: 12645-31-7

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Value: 211.3 mg/l at 25 degree C  
Method: other: WSKOW Program, version 1.36  
Year: 1999  
GLP: no  
Testsubstance: other TS: molecular structure  
Reliability: (2) valid with restrictions  
Accepted calculation method  
Flag: Critical study for SIDS endpoint  
16-OCT-2001

(1)

### 2.6.2 Surface Tension

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### 2.7 Flash Point

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### 2.8 Auto Flammability

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### 2.9 Flammability

-

### 2.10 Explosive Properties

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### 2.11 Oxidizing Properties

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### 2.12 Additional Remarks

-

## 3. Environmental Fate and Pathways

## 3.1.1 Photodegradation

Type: air  
 INDIRECT PHOTOLYSIS  
 Sensitizer: OH  
 Conc. of sens.: 1560000 molecule/cm3  
 Rate constant: .00000000328992 cm3/(molecule \* sec)  
 Degradation: 50 % after 3.9 hour(s)  
 Method: other (calculated): AOP Program (v1.89)  
 Year: 1999 GLP: no  
 Test substance: other TS: molecular structure  
 Result: ----- SUMMARY (AOP v1.89): HYDROXYL RADICALS -----  
 Hydrogen Abstraction = 32.6192 E-12 cm3/molecule-sec  
 Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec  
 Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
 Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec  
  
 OVERALL OH Rate Constant = 32.8992 E-12 cm3/molecule-sec  
 HALF-LIFE = 0.325 Days (12-hr day; 1.5E6 OH/cm3)  
 HALF-LIFE = 3.901 Hrs  
 Reliability: (2) valid with restrictions  
 Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 27-JUN-2001 (1)

## 3.1.2 Stability in Water

Type: abiotic  
 Method:  
 Year: GLP:  
 Test substance: other TS: phosphoric acid, 2-ethylhexyl ester; purity not noted  
 Remark: The method, OECD 111: Hydrolysis as a Function of pH, in Section 1, Qualifying Statements, says "This Test Guideline applies only to water soluble compounds." The method also references OECD 105: Water Solubility.  
  
 We attempted to make a water solution of CASRN 12645-31-7 (Phosphoric acid, 2-ethylhexyl ester).  
 Even at 400 ppm, the product was obviously water insoluble. A cosolvent, isopropyl alcohol, which is allowed at a <1% level was tried but did not help. Even at 40 ppm, the product does not appear to be soluble. The product is simply not water soluble enough to make a solution which could be adequately quantitated for determination of hydrolysis.  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (4)

## 3.1.3 Stability in Soil

-

## 3. Environmental Fate and Pathways

## 3.2 Monitoring Data (Environment)

-

## 3.3.1 Transport between Environmental Compartments

Type: fugacity model level III

Media:

Air (Level I):

Water (Level I):

Soil (Level I):

Biota (L.II/III):

Soil (L.II/III):

Method: other: Level III Fugacity Model

Year:

Result:	Media	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
	Air	0.000783	7.8	1000	8.41e-015
	Water	29	360	1000	1.65e-016
	Soil	70.8	360	1000	9.56e-016
	Sediment	0.188	1.44e+003	0	9.96e-017

Persistence Time: 452 hr

Reaction Time: 520 hr

Advection Time: 3.45e+003 hr

Percent Reacted: 86.9

Percent Advected: 13.1

Remark: Default input values of 1000 kg/hr were used for model.

Reliability: (2) valid with restrictions

Accepted calculation method

Flag: Critical study for SIDS endpoint

16-OCT-2001

(1)

## 3.3.2 Distribution

-

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

Remark: Two tested chemicals (107-66-4 and 78-42-2) are regarded as "not readily biodegradable" with rates < 60% in the "closed bottle" test. The trend within the closed bottle tests clearly showed that the compound is metabolized slower as it becomes more polar. Thus, one could predict that the mono-ester would not be metabolized in the "closed bottle" system. The mono-ester (#12645-31-7) is expected to be "not readily biodegradable". See IUCLID data sets on CAS#107-66-4 and 78-42-2).

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

Species: other  
Exposure period:  
Concentration:  
BCF: 21.92  
Elimination:  
Method: other: BCF Program (v2.13)  
Year: GLP: no  
Test substance: other TS: molecular structure  
Result: CHEM : Phosphoric acid, 2-ethylhexyl ester  
MOL FOR: C8 H19 O4 P1  
MOL WT : 210.21  
----- Bcfwin v2.12 -----  
Log Kow (estimated) : 2.65  
Log Kow (experimental): not available from database  
Log Kow used by BCF estimates: 2.65  
  
Equation Used to Make BCF estimate:  
Log BCF = 0.77 log Kow - 0.70 + Correction  
  
Correction(s): Value  
No Applicable Correction Factors  
  
Estimated Log BCF = 1.341 (BCF = 21.92)  
Reliability: (2) valid with restrictions  
Accepted calculation method  
27-JUN-2001 (1)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

Type: other: calculation  
 Species: other: fish  
 Exposure period: 96 hour(s)  
 Unit: mg/l Analytical monitoring: no  
 LC50: 38.164  
 Method: other: ECOSAR Program (v0.99e)  
 Year: 1999 GLP: no  
 Test substance: other TS: molecular structure  
 Result: ECOSAR Class Organism Duration End Pt mg/L (ppm)  
 =====  
 Neutral Organic SAR: Fish 14-day LC50 76.649  
 (Baseline Toxicity)  
  
 Neutral Organics: Fish 96-hr LC50 38.164  
 Neutral Organics: Fish 14-day LC50 76.649  
 Neutral Organics: Fish 30-day ChV 5.460  
 Neutral Organics: Fish(SW) 96-hr LC50 11.972  
 (ChV =chronic value)  
 Reliability: (2) valid with restrictions  
 Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001

(1)

## 4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculation  
 Species: Daphnia sp. (Crustacea)  
 Exposure period: 48 hour(s)  
 Unit: mg/l Analytical monitoring: no  
 LC50 : 42.772  
 Method: other: ECOSAR Program (v0.99e)  
 Year: 1999 GLP: no  
 Test substance: other TS: molecular structure  
 Result: ECOSAR Class Organism Duration End Pt mg/L  
 =====  
 Neutral Organics: Daphnid 48-hr LC50 42.772  
  
 Neutral Organics: Daphnid 16-day EC50 2.915  
  
 Neutral Organics : Mysid Shrimp 96-hr LC50 6.921  
 Reliability: (2) valid with restrictions  
 Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001

(1)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)  
Endpoint: growth rate  
Exposure period: 72 hour(s)  
Unit: mg/l Analytical monitoring:  
NOEC: 5  
EC50: 168  
EC90 : 207  
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"  
Year: 1992 GLP: yes  
Test substance: other TS: phosphoric acid, 2-ethylhexyl ester; purity not noted  
Result: 24 hr EC50 = 110 mg/l  
48 hr EC50 = 132 mg/l  
Test condition: test water: highly purified deionized water  
medium: OECD 201 recommended Freshwater Algal Assay medium  
pH: approx. 8  
temperature: 21.2 - 23.1 degree C  
light: 8723, 9680, 8822 lux  
Reliability: (1) valid without restriction  
GLP Guideline study  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (5)

Species: Selenastrum capricornutum (Algae)  
Endpoint: biomass  
Exposure period: 72 hour(s)  
Unit: mg/l Analytical monitoring:  
NOEC: 5  
EC50: 161  
EC90 : 198  
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"  
Year: 1992 GLP: yes  
Test substance: other TS: phosphoric acid, 2-ethylhexyl ester; purity not noted  
Result: 24 hr EC50 = 110 mg/l  
48 hr EC50 = 136 mg/l  
Test condition: test water: highly purified deionized water  
medium: OECD 201 recommended Freshwater Algal Assay medium  
pH: approx. 8  
temperature: 21.2 - 23.1 degree C  
light: 8723, 9680, 8822 lux  
Reliability: (1) valid without restriction  
GLP Guideline study  
Flag: Critical study for SIDS endpoint  
16-OCT-2001 (5)

#### 4. Ecotoxicity

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Species: other algae: green algae  
 Endpoint:  
 Exposure period: 96 hour(s)  
 Unit: mg/l Analytical monitoring: no  
 EC50: 27.759  
 Method: other: ECOSAR Program (v0.99e)  
 Year: 1999 GLP: no  
 Test substance: other TS: molecular structure  
 Result: ECOSAR Class Organism Duration End Pt mg/L (ppm)  
 =====  
 Neutral Organics: Green Algae 96-hr EC50 27.759  
 Neutral Organics: Green Algae 96-hr ChV 4.042  
 (ChV =chronic value)  
 Reliability: (2) valid with restrictions  
 Accepted calculation method  
 Flag: Critical study for SIDS endpoint  
 16-OCT-2001 (1)

#### 4.4 Toxicity to Microorganisms e.g. Bacteria

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#### 4.5 Chronic Toxicity to Aquatic Organisms

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##### 4.5.1 Chronic Toxicity to Fish

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##### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

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#### 4. Ecotoxicity

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##### TERRESTRIAL ORGANISMS

##### 4.6.1 Toxicity to Soil Dwelling Organisms

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##### 4.6.2 Toxicity to Terrestrial Plants

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##### 4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

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##### 4.7 Biological Effects Monitoring

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##### 4.8 Biotransformation and Kinetics

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##### 4.9 Additional Remarks

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## 5. Toxicity

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### 5.1 Acute Toxicity

#### 5.1.1 Acute Oral Toxicity

Remark: The acute oral LD<sub>50</sub> of 2-ethyl hexyl phosphate (12645-31-7) is expected to be about 2000 mg/kg bw in rats , which is similar to the acute toxicity of Dibutyl hydrogen phosphate (107-66-4) of same molecular weight. (See IUCLID data sets on CAS#107-66-4, 126-73-8, 298-07-7 and 78-42-2)

#### 5.1.2 Acute Inhalation Toxicity

-

#### 5.1.3 Acute Dermal Toxicity

Remark: The dermal LD50 for tributyl phosphate and tris(2-ethyl hexyl) phosphate are > 10,000 mg/kg bw. It is predicted that the acute dermal toxicity of 2-ethyl hexyl phosphate will also be in the non-toxic range. (See IUCLID data sets on CAS#126-73-8 and 78-42-2)

#### 5.1.4 Acute Toxicity, other Routes

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### 5.2 Corrosiveness and Irritation

#### 5.2.1 Skin Irritation

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#### 5.2.2 Eye Irritation

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### 5.3 Sensitization

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### 5.4 Repeated Dose Toxicity

Remark: Repeat dose studies have been conducted with three chemical members of the Phosphoric Acid Derivatives category, and demonstrate an apparent reduction in toxicity with increasing molecular weight. The toxicity of 2-ethyl hexyl phosphate (12645-31-7) is expected to be similar to the toxicity of Dibutyl hydrogen phosphate (107-66-4) of same molecular weight. The 44 day oral exposure NOAEL of Dibutyl hydrogen phosphate is 30 mg/kg bw in rats. (See IUCLID data sets on CAS#107-66-4, 126-73-8, and 78-42-2)

5. Toxicity

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## 5.5 Genetic Toxicity 'in Vitro'

Remark: The weight of evidence for the members of the Phosphoric Acid Derivatives category indicates these chemicals are not mutagenic or clastogenic. (See IUCLID data sets on CAS#107-66-4, 126-73-8, 298-07-7, and 78-42-2)

## 5.6 Genetic Toxicity 'in Vivo'

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## 5.7 Carcinogenicity

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## 5.8 Toxicity to Reproduction

Remark: Adequate reproductive and developmental studies are available for the two similar chemicals (107-66-4 and 126-73-8). These studies indicate an absence of reproductive or developmental effects of these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, no reproductive or developmental effects of 2-ethyl hexyl phosphate (12645-31-7) is expected at doses ranging from >225 to 1000 mg/kg. (See IUCLID data sets on CAS#107-66-4 and 126-73-8)

## 5.9 Developmental Toxicity/Teratogenicity

Remark: Adequate reproductive and developmental studies are available for the two similar chemicals (107-66-4 and 126-73-8). These studies indicate an absence of reproductive or developmental effects of these chemicals at doses ranging from >225 to 1000 mg/kg. Since repeat dose testing of this category demonstrates an apparent reduction in toxicity with increasing molecular weight, no reproductive or developmental effects of 2-ethyl hexyl phosphate (12645-31-7) is expected at doses ranging from >225 to 1000 mg/kg. (See IUCLID data sets on CAS#107-66-4 and 126-73-8)

## 5.10 Other Relevant Information

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## 5.11 Experience with Human Exposure

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## 6. References

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- (1) Meylan W. and Howard P. (1999) EPIWin Modeling Program.  
Syracuse Research Corporation. Environmental Science Center,  
6225 Running Ridge Road, North Syracuse, NY 13212-2510
- (2) Uniqema data
- (3) Crompton MSDS
- (4) Baker Petroloite Corporation. Analytical Services. January, 2001.
- (5) Environmental Services Group, Baker Petrolite Corporation,  
Missouri, USA. April, 2001.

## 7. Risk Assessment

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### 7.1 End Point Summary

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### 7.2 Hazard Summary

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### 7.3 Risk Assessment

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